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NUMERICAL AND ANALYTICAL SOLUTIONS OF DISPERSION PROBLEMS IN HOMOGENEOUS AND LAYERED AQUIFERS

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Cambridge, Massachusetts

May 1966

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by

Uri Y. Shamir and Donald R. F. Harleman

HYDRODYNAMICS LABORATORY

Report No. 89

Prepared Under
Division of Water Supply and Pollution Control,
Public Health Service, National Institutes of Health,
U.S. Department of Health, Education and Welfare
under Research Grant WP-00711

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ABSTRACT

From a review of previous work on dispersion in porous media it is concluded that at present the tools for solving most practical problems of mixing of fluids in artificial recharge, waste water disposal and ground water contamination are still missing. Available analytical solutions are applicable to simple cases only, and numerical methods which have been developed are not efficient enough to be used in practice.

A numerical method is proposed for the solution of dispersion problems in steady three-dimensional potential flow fields in porous media, in which the miscible fluids have the same density and viscosity. The method is developed and tested for two-dimensional problems, and the extension to three dimensions is presented.

The numerical scheme uses the convective dispersion equation in curvilinear coordinates consisting of the flow streamlines and equipotentials. By means of this equation any problem of dispersion in a steady potential flow field, as well as a special type of problems with unsteady flow, can be solved. The scheme uses the most efficient method available for treating convection and dispersion in the direction of the flow, the Stone and Brian method, and an alternating direction procedure for treating the dispersion at right angles to the streamlines.

The numerical scheme is programmed for a computer and applied to a few simple cases, for which analytical solutions exist. The experience gained is then applied to a few practical, and more complex, problems.

Analytical solutions are obtained for two problems of dispersion in layered porous media:

a. Longitudinal dispersion in flow perpendicular to the layers, and

b. Lateral dispersion in flow parallel to the layers.

Experiments are described for the verification of the analytical results. Results obtained from the numerical scheme for these cases are compared with experimental results and theory.

A description of the computer programs, flow charts and listings are included.

Suggestions for further extensions and applications of the numerical scheme are included in the closing chapter.

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Many constructive suggestions concerning the numerical work were made by Professor P.L.T. Brian of the Department of Chemical Engineering at M.I.T.

Mr. R.B. Lantz, of the Esso Production Research Company, kindly supplied some information which is included in Chapter II.

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All the computer work was conducted at the Computation Center at M.I.T. The assistance of its staff is gratefully acknowledged.

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I. INTRODUCTION

The Civil Engineer's interest in the study of dispersion in porous media stems from water quality problems such as sea water intrusion into coastal aquifers, recharge of surface water into underground storage, waste water disposal and pollution of ground water by infiltration from streams and rivers. Ground water is playing an ever increasing role in the water resources schemes of many regions, and the use of aquifers as operative reservoirs is becoming more common. Efficient use of aquifers as reservoirs requires the ability to predict the patterns of mixing of the recharged water with the native water. Usually the recharged water is of a quality not acceptable for use, and only after adequate dilution by mixing with fresh water in the aquifer can it be pumped out for consumption.

This interest has spurred the investigation of dispersion in porous media on two levels. On the one hand basic studies were conducted to explain the underlying physical laws, and on the other field studies were carried out to get answers for specific problems.

The basic studies resulted in analytical solutions to the problems of longitudinal and lateral dispersion in homogeneous-isotropic(*) porous media. Some approximate solutions have been obtained for other two dimensional geometries of the flow field, e.g. radial flow and source-sink flow in homogeneous-isotropic media. The governing equations for dispersion in homogeneous-anisotropic porous media have been obtained, but no specific solutions exist. The experimental work resulted in correlations of the longitudinal and lateral dispersion coefficients with the seepage velocity and properties of the media and the fluid.

(*) Homogeneous - a medium in which the geometric properties are invariant under translation of the coordinate axes.
Isotropic - a medium in which the geometric properties are invariant under rotation of the coordinate axes.

Much remains to be done in applying the results obtained in the laboratory to field situations. Natural aquifers are usually non-homogeneous and anisotropic. Flows are often unsteady and of complex geometry.

The ultimate goal of any research in the field of Engineering is the ability to give answers to practical problems, and the present investigation is a step in this direction.

II. LITERATURE REVIEW AND OBJECTIVES

2.1 Review of Previous Work

Work on flow of miscible fluids in porous media has been carried out by Civil, Chemical and Petroleum engineers. There have been four major parts to this effort:

a. The equations describing hydrodynamic dispersion have been derived, and analytical solutions were obtained for a few simple cases.

b. Experimental work has been conducted to verify theoretical results, and obtain the magnitude of the dispersion coefficients.

c. The results were used to obtain answers to specific field problems, and

d. Numerical solutions were sought for both the basic cases and for more complex geometries and flow conditions.

The differential equations describing dispersion in homogeneous-isotropic porous media were derived by two different approaches. Most of the investigators have used a mass balance approach. The equation for conservation of mass of the dispersing material in an elementary control volume equates the rate of accumulation of mass inside the volume to the net influx of mass through the boundaries of the element. The net influx is made up of convective terms and terms involving dispersion. The tracer material is usually considered inert. No chemical reactions take place in the fluid phase, the tracer does not decay with time, and adsorption to the surface of the solid phase is neglected. The molecular diffusion of the tracer in the fluid phase is neglected in most equations as compared with hydrodynamic dispersion. It is included, however, when the velocities are small and molecular diffusion may have some effect.

The term "dispersion coefficient" in this work refers only to that part resulting from hydrodynamic dispersion. When molecular diffusion is included the coefficients will be called total dispersion coefficients.

The other approach is called statistical. The motion of an individual fluid particle is considered as made up of a large number of steps. At each step some parameters of the particle's motion, such as its velocity or direction are determined from a probability distribution function. Danckwerts [20] used this approach in 1953. Scheidegger [50], [51] gave a general discussion of the method, and Saffman [48] used a random residence time model.

Bachmat and Bear [1] present the general equations of dispersion in homogeneous-isotropic porous media. Their equations result from the mass balance approach. The general form of the dispersion equation in Cartesian coordinates is

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ik}\frac{\partial C}{\partial x_k} - u_i C\right) \qquad (2\text{-}1)$$

where C = concentration of dispersing mass

x_i (i = 1, 2, 3) = Cartesian coordinates

u_i = seepage velocity in direction i

D_{ik} = components of the "factor of dispersion", a second rank symmetric tensor, which does not include the molecular diffusivity.

Bear [4] concluded from physical considerations that the factor of dispersion is the inner product of a dispersivity tensor $a_{ik\ell m}$, which is a function of the geometry of the media, and the tensor $u_\ell u_m/|\underline{u}|$, where $|\underline{u}|$ is the magnitude of the velocity vector. For a homogeneous-isotropic medium this leads to the relations

$$D_L = \alpha_L\, u \qquad (2\text{-}2)$$

and

$$D_T = \alpha_T\, u \qquad (2\text{-}3)$$

D_L and D_T are the longitudinal and lateral (transverse) dispersion coefficients, respectively, (dimension L^2/T). α_L and α_T are the longitudinal and lateral dispersivities, respectively (dimension L).

Experimental results for both D_L and D_T are usually given in one of the forms

$$D = \alpha_1 \, u^{\beta_1} \tag{2-4}$$

$$\frac{D}{\nu} = \alpha_2 \left(\frac{u \, d_{50}}{\nu}\right)^{\beta_2} \tag{2-5}$$

$$\frac{D}{\nu} = \alpha_3 \left(\frac{u \sqrt{k}}{\nu}\right)^{\beta_3} \tag{2-6}$$

where d_{50} = the mean grain size of the medium
k = the intrinsic permeability of the medium (dimension L^2)
ν = kinematic viscosity of the fluid
α's and β's = experimentally determined coefficients.

There is a large variation in the values of these coefficients as reported by different investigators. The variation is due to differences in experimental techniques, most important among these is the method of measuring concentrations. This is discussed in more detail in Section 5.3.1.

The reported values of β_1 for the longitudinal dispersion coefficient, D_L, are larger than 1.0, and go up to 1.2. Mohtadullah [37] has shown that β_1 depends on the uniformity of the medium. For a uniformity coefficient ($UC = d_{60}/d_{10}$) of 1.25, $\beta_1 = 1.2$, and it decreases with decrease in uniformity to $\beta_1 = 1.02$ for UC = 6.0. Experimental results for longitudinal dispersion are given by Banks and Ali [2], Bear [5], Blackwell [9], Cairns and Prausnitz [12], Carberry and Bretton [13], Ebach and White [23], Harleman, Mehlhorn and Rumer [29], Hoopes and Harleman [32] and others. For lateral dispersion the data is scarcer. Results are given by Blackwell [9], Grane and Gardner [26], Harleman and Rumer [28], Hoopes and Harleman [32], Simpson [55] and Van der Poel [61]. A compilation of experimental results for both longitudinal and lateral dispersion is given by Perkins and Johnston [42].

The relations (2-2) and (2-3) are often used in theoretical considerations, because it simplifies the analysis. The relations are also fairly representative of the experimental results.

Bachmat and Bear [1] give another useful form of the dispersion equation in curvilinear coordinates consisting of the streamlines and equipotentials (hereafter called the Φ-ψ coordinate system). Hoopes and Harleman [32] give this equation for two-dimensional flow in homogeneous-isotropic media in the form

$$\frac{\partial C}{\partial t} + q^2 \frac{\partial C}{\partial \Phi} = q^2 \frac{\partial}{\partial \Phi} \left[(\alpha_L q + D_m) \frac{\partial C}{\partial \Phi} \right] + q^2 \frac{\partial}{\partial \psi} \left[(\alpha_T q + D_m) \frac{\partial C}{\partial \psi} \right] \tag{2-7}$$

where q is the seepage velocity along the streamline, and D_m is the molecular diffusivity (dimension L^2/T). Equations (2-2) and (2-3) are assumed to hold in the derivation of equation (2-7). D_m is added because there may be parts of the flow field where q is very small and the mixing is governed partly by molecular diffusion.

For a unidirectional flow, in the x-direction, equation (2-1) becomes

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D_L \frac{\partial^2 C}{\partial x^2} + D_T \frac{\partial^2 C}{\partial y^2} \tag{2-8}$$

where u, D_L and D_T are constants.

When there is no lateral variation in concentration the equation describes longitudinal dispersion

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D_L \frac{\partial^2 C}{\partial x^2} \tag{2-9}$$

Ogata and Banks [39] give an analytical solution of equation (2-9) for a step input of concentration. An analytical solution for an input concentration which is a periodic function of time is presented by Ebach and White [23].

There is no known solution of equation (2-8). Harleman and Rumer [28] treat one case described by this equation in which the term involving longitudinal dispersion may be neglected compared with the other terms. They consider the steady state concentration distribution resulting from the input

$$C(0,y) = C_0 \qquad - \infty < y \le 0$$

$$C(0,y) = 0 \qquad 0 < y < \infty$$

and show that the second derivative of the concentration with respect to x is so small as to make the whole term negligible (even though D_L is in the order of 10 - 20 times D_T). The reduced equation for the steady state is

$$u \frac{\partial C}{\partial x} = D_T \frac{\partial^2 C}{\partial y^2} \tag{2-10}$$

The convective dispersion equation has been used in other coordinate systems for particular problems. A cylindrical coordinate system was used by Ebach and White [23] and Hoopes and Harleman [32] for axial flow with longitudinal and lateral concentration gradients. Hoopes and Harleman [32] treat the problem of dispersion in radial flow from a single well fully penetrating a confined aquifer made of a homogeneous-isotropic porous medium, of thickness b and porosity θ. The convective-dispersion equation in cylindrical coordinates is one dimensional

$$\frac{\partial C}{\partial t} + \frac{A}{r}\frac{\partial C}{\partial r} = \alpha_L \frac{A}{r}\frac{\partial^2 C}{\partial r^2} \tag{2-11}$$

where $A = \frac{Q}{2\pi \; b\theta}$

Q = the well discharge.

An approximate solution of equation (2-11) was obtained for the case of a step input of concentration (see Section 4.3 for further details).

Only a few other flow fields with dispersion have been treated. Hoopes and Harleman [32] treat dispersion in flow between two wells fully penetrating a confined aquifer of homogeneous-isotropic media, one pumping and the other recharging at the same rate Q. The convective dispersion equation is used in Φ-ψ coordinates. The full equation cannot be solved analytically due to the variable coefficients, and three approximate solutions were obtained:

a. no dispersion, i.e. $\alpha_L = \alpha_T = 0$.

b. no lateral dispersion, i.e. $\alpha_T = 0$, $\alpha_L \neq 0$.

c. no longitudinal dispersion, i.e. $\alpha_L = 0$, $\alpha_T \neq 0$.

In many practical problems involving the flow of two miscible fluids through porous media dispersion is neglected. The fluids are considered immiscible, and the time history of concentration at any point in the flow field is a result of a "piston-flow" along each streamline. Bear and Jacobs [6] treated the problem of a well fully penetrating a confined aquifer of homogeneous-isotropic media, in which there exists a unidirectional flow. The well intermittantly recharges, pumps or is idle. They treat the recharged water and the water flowing in the aquifer as immiscible, and get curves for the relative concentration in the water pumped from the well for different conditions.

Harpaz and Bear [31] discuss the dispersion in flow from a single or several wells in a confined aquifer. A few field tests are presented for a single well recharging into a phreatic aquifer and then pumping from it.

A computer program for predicting waste water transport by ground water is described by Nelson [80]. Dispersion is not included, and the propagation of the concentration front is considered as a "piston flow" in each streamtube.

No solutions have been found in the literature on dispersion in non-homogeneous and anisotropic media. The convective dispersion equation for homogeneous-anisotropic media is given by Bear and Bachmat [6], but no solutions have been obtained. The only case of non-homogeneity that was treated in past work is that of a random permeability distribution used in Peaceman and Rachford's numerical scheme [83].

Many investigators have resorted to numerical solutions of the convective dispersion equation for a specific problem when no analytical solution could be found. The differential equation was replaced by an explicit finite difference equation (see Chapter III). The size of the grid spacing and the time increment for an explicit scheme are restricted to very small values by a stability criterion, and this makes the numerical scheme impractical in terms of computer time requirement. In a few cases the exact differential equation was first simplified, using some assumptions about the relative importance of the different terms in it. Exact, and sometimes only approximate, solutions were obtained for the simplified equation. A numerical solution by an explicit scheme was calculated, to verify the validity of the assumptions and the analytical solution.

Hoopes and Harleman [32] obtained a numerical solution by an explicit scheme for the radial flow and the two-well problem. A numerical solution for the two-well problem was obtained only for the case in which lateral dispersion was neglected. An attempt was made to solve the full equation but it was fount that the computer time required was too large, so the solution was not carried to completion. Some details about these results, and the computer time required to obtain them, are presented in Sections 4.3 and 4.5.

Systematic work on devising general numerical methods for solving problems of miscible displacement has been done mostly by investigators in the Petroleum industry. Different types of fluids are used to force oil into pumping wells. The expendable "driving" fluid (usually water or hydrocarbons) is recharged into the oil field to create gradients which increase the flow of the oil into the recovery well. Here both viscosity and density differences between the fluids, as well as dispersion, play an important role. The problem has to be solved by coupling a flow equation (Darcy's law) for each fluid with a dispersion equation.

Displacement processes in oil recovery may be miscible or immiscible, depending on the driving fluid. Both cases have been treated numerically. The immiscible case was solved first, and the results were used in solving the more complex miscible case.

In 1959, Douglas, Peaceman and Rachford [73] solved the problem of immiscible displacement. They combined the Darcy equation with the continuity equation for each fluid component. They considered a two-dimensional flow and used an alternating direction scheme. (This scheme, originally proposed by Peaceman and Rachford [82], is discussed in Section 3.3.)

Peaceman and Rachford [83] used Darcy's law for each fluid and a dispersion equation in Cartesian coordinates for a two-dimensional flow of miscible fluids. At each time step the distribution of pressure in the flow field is obtained from the equation describing the flow of each fluid. With this pressure distribution the new flow field can be determined, that is, the velocity at each point can be computed. Using these velocities the new concentration distribution for the next time step may be computed from the convective dispersion equation, used in the form of equation (2-8). The finite difference analogue of the convective dispersion equation is centered in time. The convective term includes for each grid point the velocities at all adjacent grid points. The resulting set of equations has five unknowns per row. The solution of this set is done by iterations.

The authors consider two alternatives for weighting the convective terms at adjacent grid points, one is centered in space while the other is backward in space. They compare the results of the two schemes for the one dimensional case with no viscosity or density differences. They use equation (2-9) with a step input, and compare the numerical results with the analytical solution. They conclude that each of the proposed alternatives for weighting of the convective terms gives better results than the other for some region of the solution. The final scheme uses one weighting scheme in the immediate vicinity of the advancing dispersed front, and the other scheme over the rest of field.

In 1964 Gardner, Peaceman and Pozzi [77] used the method of characteristics to improve the numerical solution of the same problem. This scheme is also referred to as the "Particle in Cell" method. In addition to the usual division of the two-dimensional space into rectangles by grid lines they introduce a set of moving points. Each moving point has associated with it a concentration, which varies with time. The velocities at each time step are obtained by the method given by Peaceman and

Rachford [83]. Each moving point is then moved to a new location using the local velocity and the time increment. Each rectangle of the grid is assigned a new concentration equal to the average of the concentrations of the moving points in it. This concentration in each rectangle is modified by dispersion in two dimensions, and the change in concentration is then applied to all moving points within the rectangle.

This method prevents numerical dispersion. Numerical dispersion is an effective dispersion caused by the finite difference approximation. It produces dispersion in the results even when the (physical) dispersion coefficients are set equal to zero. The method of characteristics assures that a sharp front will maintain its shape throughout the solution in the absence of physical dispersion.

The authors test their scheme for the same one-dimensional case as Peaceman and Rachford [83]. They conclude that their method is an improvement, and can handle any value of the dispersion coefficient. Two moving points per grid rectangle are sufficient, and increasing this number does not improve the accuracy.

In a private communication Mr. R.B. Lantz, of the Esso Production Research Company, has supplied the following information concerning computer time required to obtain some of the results presented in the paper:

a. The solution of the two-dimensional concentration equation, equation (9) in the paper, for 40 x 20 grid points, required an average of 30 seconds per time step on an IBM 7044. This is in addition to 25 seconds per time step for the solution of the pressure equation for the same case.

b. The solution of the one-dimensional convective dispersion equation with no density or viscosity differences, equation (15) in the paper, for 48 grid points, required less than 3 seconds per time step on an IBM 7044.

Stone and Brian [86] made a thorough analysis of a numerical scheme to solve equation (2-9). They use six points, involving three adjacent space locations at two time levels. They assign arbitrary weighting coefficients in the convective and time terms, and determine their magnitude so that the numerical solution approaches the analytical solution. They also propose an iterative scheme with three cycles per time step to improve the solution. A detailed description of their method is given in Section 3.2.

Stone and Brian's method requires much less computer time and storage than the method of characteristics, because one does not have to deal with the moving points which are used in the latter. The one-dimensional problem solved by Gardner, Peaceman and Pozzi [77] was computed by the Stone and Brian scheme for comparison. The same data was used, with 48 slices, three cycles, and the same time increment. The results had the same degree of accuracy as those presented in [77], and computation time used was 0.54 seconds per time step. Thus, even without solving the pressure equation, the method of characteristics requires five times as much computer time.

To make a complete and fair comparison of the methods one has to compare the results of each scheme, used at its maximum efficiency, for a wide range of problems. This could not be done with the information that was available about the method of characteristics. It seems reasonable to say, however, that Stone and Brian's scheme requires less computer time and storage space than the best scheme previously suggested, in the absence of viscosity or density differences.

The accuracy of the Stone and Brian scheme is of the same order of the accuracy achieved by the method of characteristics. The only case in which the latter method has some advantage (for the one dimensional problem) is when $D_L = 0$.

For the one-dimensional case of no density and viscosity differences between the miscible fluids the Stone and Brian scheme is a substantial improvement over other numerical schemes. Problems of dispersion in artificial recharge and waste disposal operations usually involve miscible fluids with little or no density and viscosity differences, in flow fields which are usually two- or three-dimensional. A numerical scheme which incorporates the advantages of the Stone and Brian scheme, and is general enough to handle two- and three-dimensional problems would be a useful tool in solving practical problems. It is one of the purposes of this work to develop such a numerical scheme.

2.2 Objectives of the Present Work

It is clear from the previous section that the area in which least has been done in the past is the application of the basic results to field conditions. Practical problems involve complex flow geometries in media which are usually neither isotropic nor homogeneous. Solutions to more complex problems are needed. More important is finding a general method for solving practical problems. Such a method could be found in one of the numerical schemes for two dimensional problems, e.g. the method of characteristics. These schemes treat a case which is more general than the one considered in this work, namely that involving density and viscosity differences. The price paid for this generality is in computation time needed to solve the problem. A substantial gain in efficiency can be achieved by a different numerical scheme, if only cases with no density and viscosity differences are considered. Such an improvement may turn academic results into a practical tool. At the same time the ability to solve complex problems will allow the effort to be concentrated in studying more basic problems, such as the question of the validity of equations (2-2) and (2-3) for unsteady and non-uniform flows.

The objectives of this work are to:

a. Develop a numerical technique for the solution of dispersion problems in two-dimensional, steady flow fields with no density and viscosity differences between the mixing fluids. The scheme is then tested in some simple cases for which exact or approximate solutions are available. It is also applied to a few, more complex, cases.

b. Obtain analytical solutions for two problems of dispersion in non-homogeneous porous media. Experiments are described, which verify the theory. Results of the proposed numerical scheme for these cases are compared with theory and experiments.

III. NUMERICAL SOLUTIONS

3.1 Introduction and Basic Concepts

This chapter assumes some previous knowledge of numerical solutions for differential equations. Nevertheless a few of the basic concepts will be presented and explained to make this chapter somewhat self contained.

To solve a differential equation numerically it is replaced by a difference equation in which the derivatives are expressed as finite differences. If the exact solution of the differential equation is denoted by S, and the exact solution of the difference equation is denoted by D, $|S - D|$ is called the Truncation error. This error is due to the form of the difference equation and to the finite mesh size. The solution of the difference equation is usually carried out on a computer. If the numerical solution is denoted by N, then $|D - N|$ is the numerical error. It is caused by the finite accuracy of the machine performing the operations. The numerical error is often called the Roundoff error.

The conditions for Convergence of a finite difference scheme are those for which $|S - D| \to 0$ over the whole region of the solution. The conditions of Stability of a finite difference scheme are those for which $|D - N| \to 0$ over the whole region of interest.

The problem is to find N such that $|S - N|$ is smaller than some error criterion over the whole region of the solution. $(S - N)$ may be expressed as

$$(S - N) = (S - D) + (D - N)$$

so that the total error is made up of the truncation error and the roundoff error. It is interesting to note that it is often the truncation error which constitutes the larger part of the total error.

This work deals with initial value problems of parabolic differential equations. The region of space in which a solution is sought is either finite or semi infinite. For the finite region, in addition to the initial condition, some information about the value of the function is needed on all boundaries at all times. For the semi infinite region in space there is in addition to the initial condition and boundary conditions on the finite boundaries some condition on the function or its derivatives as the space variables approach infinity.

To present some general ideas about numerical solutions for problems of the type described above the one dimensional linear convective dispersion is used

$$- D_L \frac{\partial^2 C}{\partial x^2} + u \frac{\partial C}{\partial x} + \frac{\partial C}{\partial t} = 0 \qquad (3\text{-}1)$$

in which D_L and u are constants.

The x-axis is divided by I points into (I -1) increments, each of some length Δx. The time is divided into increments Δt. Δx and Δt may be variables. The spacing of grid points along the x-axis may be varied to create a higher density of grid points in regions where C changes rapidly with x. Δt may be varied in the progress of the solution to increase computational efficiency, while maintaining the desired accuracy. These points will be discussed again in Section 3.4, in connection with the proposed numerical scheme. In the following discussion Δx is assumed constant, but Δt is allowed to vary in the progress of the solution.

The concentration at the point $x = i\ \Delta x$ at time $t = \sum_{1}^{n} \Delta t$ (hereafter referred to as "time level n") is denoted by $C_{i,n}$.

One possible way of writing a finite difference analogue of equation (3-1) is

$$- D_L \left[\frac{C_{i+1,n} - 2C_{i,n} + C_{i-1,n}}{(\Delta x)^2}\right] + u \left[\frac{C_{i+1,n} - C_{i-1,n}}{2\Delta x}\right] +$$

$$+ \frac{C_{i,n+1} - C_{i,n}}{\Delta t} = 0 \qquad i = 1, \cdots , I \qquad (3\text{-}2)$$

This scheme is called Explicit, because the equation for each (i) includes only one unknown, $C_{i,n+1}$, for which equation (3-2) can be solved explicitly. The concentration distribution at time level (n+1) is calculated, one point at a time, from three known values at time level (n).

The explicit solution may be represented graphically by the following sketch

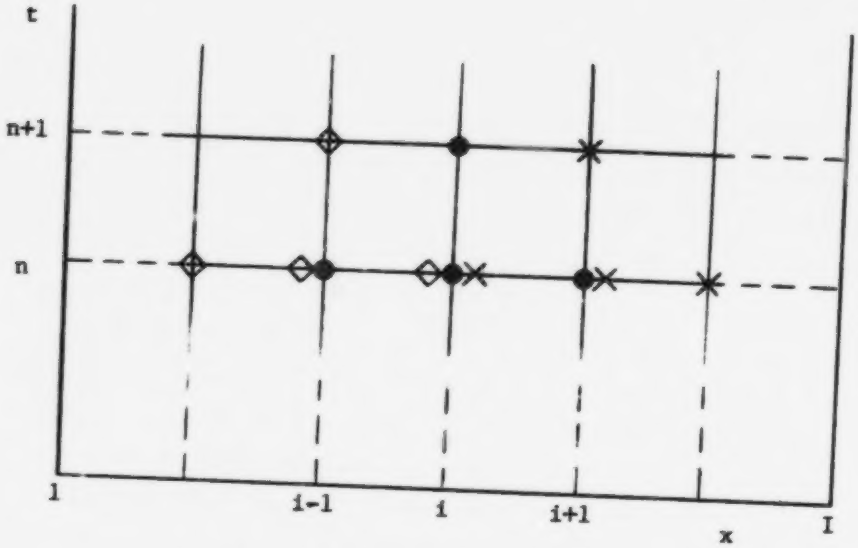

Fig. 3-1: The Explicit Scheme

where each of the equations given by (3-2) involves concentrations at four points, denoted by a common symbol. The explicit scheme is also called a forward (in time) solution. The solution begins with the given initial condition $C_{i,0}$ $i = 1, \cdots, I$, and is propagated in time by solving for C_{n+1} from C_n.

The convective term in equation (3-2) is "centered in space". Other difference analogues of the convective term, using only values of C at time level n, may be represented by the general form

$$u \left[\mu \frac{(C_{i+1,n} - C_{i,n})}{\Delta x} + (1 - \mu) \frac{(C_{i,n} - C_{i-1,n})}{\Delta x} \right] \quad (3\text{-}3)$$

where $0 \leq \mu \leq 1$. In equation (3-2) $\mu = 1/2$.

It may be shown that the stability of any finite difference analogue of equation (3-1) is determined by its form, the initial condition, and the values of the parameters $u\Delta t/\Delta x$ and $D_L\ \Delta t/(\Delta x)^2$.

When equation (3-2) is solved for $C_{i,n+1}$ we get

$$C_{i,n+1} = C_{i-1,n}\left[\frac{D_L\ \Delta t}{(\Delta x)^2} + \frac{u\Delta t}{\Delta x}\right] + C_{i,n}\left[1 - \frac{2D_L\Delta t}{(\Delta x)^2}\right]$$

$$+\ C_{i+1,n}\left[\frac{D_L\ \Delta t}{(\Delta x)^2} - \frac{u\Delta t}{\Delta x}\right] \qquad (3\text{-}4)$$

If the initial condition is considered an arbitrary function, which includes an infinite number of components with different frequencies, it can be shown that the conditions for stability of equation (3-4) lead to the restriction

$$\frac{D_L\ \Delta t}{(\Delta x)^2} \leq \frac{1}{2} \qquad (3\text{-}5)$$

If the accuracy of the decay factor at any time step is to be of order (Δt), this requires that $u\Delta t/\Delta x$ be made less than unity. Combining this with equation (3-5) leads to the approximate inequality

$$\Delta x \lesssim \frac{2D_L}{u} \qquad (3\text{-}6)$$

Condition (3-6) restricts the maximum spatial mesh size to be used. In units of (cm) and (sec) the ratio D_L/u is of the order (10^{-1}) so that Δx is restricted to values in the order of a single grain size. If equality is used in equation (3-6) then equation (3-5) may be written as

$$\Delta t \leq \frac{(\Delta x/4)}{u} \qquad (3\text{-}5a)$$

The maximum admissible time step is thus of the order of the time required by the mean velocity to cover a distance equal to a fraction of a grain size. These restrictions lead to a large amount of computation time required for even the simplest problems. Although the solution of the explicit scheme is simple, the large amount of computer time required to perform it usually renders the whole method impractical.

The restrictions on the spatial and temporal mesh size may be viewed as the result of solving at each point for $C_{i,n+1}$ separately, "uncoupled" from the values of the function at the neighboring points at the new time level. It is clear that $C_{i,n+1}$ depends not only on the values of C_{i-1} and C_{i+1} at time level (n), but also at time level (n+1). If the latter is not considered, the solution has to be propagated in the time-space domain with steps small enough to keep any small errors from growing with time (which is another way of defining stability).

Another possible finite difference analogue of equation (3-1) is

$$- D_L \left[\frac{C_{i-1,n+1} - 2C_{i,n+1} + C_{i+1,n+1}}{(\Delta x)^2}\right] + u \left[\frac{C_{i+1,n+1} - C_{i-1,n+1}}{2\Delta x}\right]$$

$$+ \frac{C_{i,n+1} - C_{i,n}}{\Delta t} = 0 \qquad i = 1, \cdots , I \qquad (3\text{-}7)$$

This is an Implicit scheme. There are three unknowns in equation (3-7) for each (i). It is written for all i and the resulting set of equations is solved simultaneously. The graphical representation of equation (3-7) is

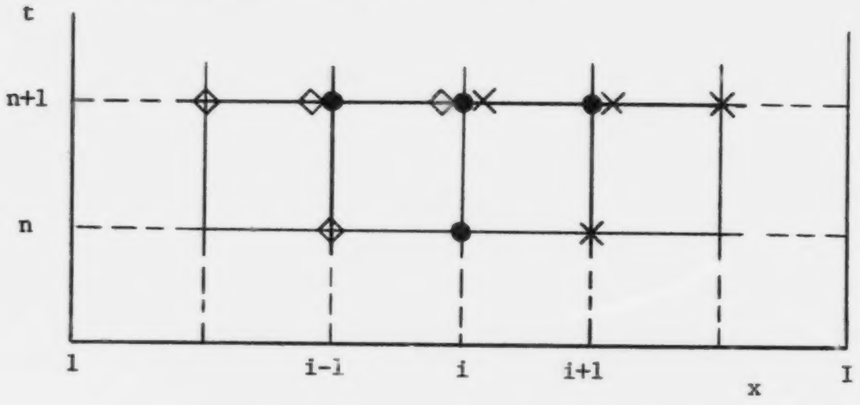

Fig. 3-2: The Implicit Scheme

At the boundary points i = 1 and i = I one must have some information about C_1 and C_I at all time levels. This is given by the boundary conditions. The treatment of different types of boundary conditions will be described in Section 3.5, in connection with the proposed numerical scheme.

The matrix of coefficients for the simultaneous equations resulting from equation (3-4) is tri-diagonal, i.e. it has only three non-zero terms per row, one on the main diagonal and one on either side of it. The first and last rows have only two non-zero elements, the third one is eliminated using the boundary conditions. The solution for a tri-diagonal matrix is achieved by successive eliminations between rows. There exists a very efficient computational algorithm for the solution, called the Thomas Algorithm. It is presented in Section 3.5.6.

The spatial derivatives in equation (3-7) are all at time level (n+1), and the time derivative is "backward" in time. Again more general forms of the spatial derivatives could be used, such as given by (3-3) for the convective term. One can also use values at both time levels. A general form for the second derivative is

$$- D_L \left[\varepsilon \left(\frac{C_{i-1,n+1} - 2C_{i,n+1} + C_{i+1,n+1}}{(\Delta x)^2} \right) + (1 - \varepsilon) \left(\frac{C_{i-1,n} - 2C_{i,n} + C_{i+1,n}}{(\Delta x)^2} \right) \right] \qquad (3\text{-}8)$$

where $0 \leq \varepsilon \leq 1$. Different values of ε give

$\varepsilon = 0$	Forward difference
$\varepsilon = 1$	Backward difference
$\varepsilon = 1/2$	Centered in time. This is called the Crank-Nicholson approximation of the second derivative.

An abbreviated notation will be used hereafter for the finite difference analogue of the second derivative, defined by

$$\Delta_x^2 (C_n) \equiv \frac{C_{i-1,n} - 2C_{i,n} + C_{i+1,n}}{(\Delta x)^2} \qquad (3\text{-}9)$$

Thus the abbreviated form of equation (3-8) is

$$- D_L [\varepsilon \Delta_x^2 (C_{n+1}) + (1 - \varepsilon) \Delta_x^2 (C_n)] \qquad (3\text{-}8a)$$

Equation (3-7) is unconditionally stable, i.e. there is no restriction on the maximum spatial mesh size or on the time step. This implies that small errors do not increase with time, but does not guarantee that the numerical solution approaches the true solution. The truncation error increases with increase in the space increment and time step, so the criterion for their maximum size is the desired accuracy. The restrictions are applied again to the parameters $u\Delta t/\Delta x$ and $D_L\Delta t/(\Delta x)^2$.

The analysis shows that the accuracy of the numerical solution for a fixed mesh size and time step depends on the frequency distribution of components in the spatial variation of the initial condition and the temporal variation of the boundary condition (i.e. on the frequencies appearing in a Fourier decomposition of these functions). When only the first few harmonics are present, that is the functions are smooth and vary slowly, $u\Delta t/\Delta x$ may be large. When there are steps in the initial or boundary conditions $u\Delta t/\Delta x$ must be restricted to small values.

The nature of the dispersion process is such that any sharp front is smeared out with time. When a step occurs, $u\Delta t/\Delta x$ may be made small initially, and then increased as the front is dispersed and smoothed. Such a procedure is used in the proposed numerical scheme, and is presented in Section 3.5.5.

It is now possible to present a numerical scheme for the solution of equation (3-1), which is one of the ingredients of the proposed numerical scheme.

3.2 Stone and Brian's Method for the One Dimensional Case

Stone and Brian [86] proposed a general weighted finite difference analogue of equation (3-1). Written in notation consistent with this work their equation (equation (13) in the paper) is

$$- D_L \left[\Delta_x^2 \frac{(C_{n+1} + C_n)}{2} \right] + \frac{u}{\Delta x} \left[a_1 \, (C_{i+1,n} - C_{i,n}) \right.$$

$$+ a_2 \, (C_{i,n} - C_{i-1,n}) + a_3 \, (C_{i+1,n+1} - C_{i,n+1})$$

$$\left. + a_4 \, (C_{i,n+1} - C_{i-1,n+1}) \right] + \frac{1}{\Delta t} \left[b_1 \, (C_{i,n+1} - C_{i,n}) \right.$$

$$\left. + b_2 \, (C_{i+1,n+1} - C_{i+1,n}) + b_3 \, (C_{i-1,n+1} - C_{i-1,n}) \right] = 0 \qquad (3\text{-}10)$$

a_1 to a_4 are arbitrary weighting coefficients of the convective term, subject to

$$a_1 + a_2 + a_3 + a_4 = 1 \qquad (3\text{-}11a)$$

and b_1 to b_3 are arbitrary weighting coefficients of the time term, subject to

$$b_1 + b_2 + b_3 = 1 \qquad (3\text{-}11b)$$

The Crank-Nicholson approximation is used for the second derivative. This scheme involves three spatial points at two time levels. Its graphical representation is

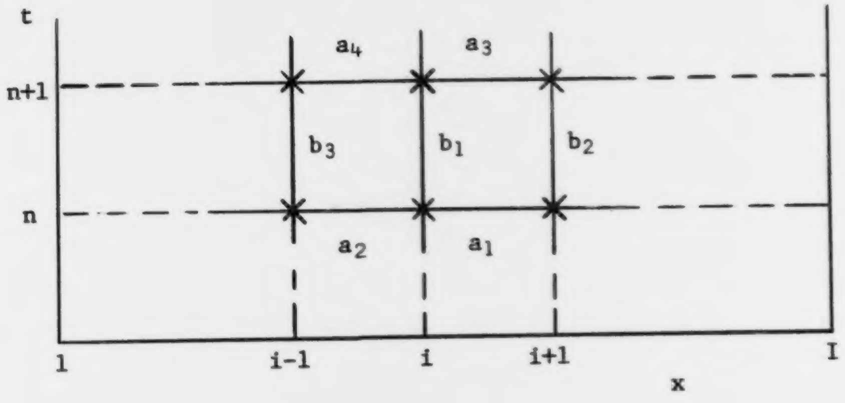

Fig. 3-3: Stone and Brian's Scheme

The initial condition is represented by a Fourier Sine series in the space variable x, with an infinite number of frequencies. The exact solution of equation (3-1) is then

$$C(x,t) = \sum_{\omega=1}^{\infty} A_\omega \cdot \exp\,(-\omega^2\pi^2 D_L t)\cdot \sin \omega\pi(x - ut) \qquad (3\text{-}12)$$

where ω is the angular frequency, and A_ω is a constant. It is seen that all components, independent of their frequency, travel with the velocity u, but each is decayed in time at a rate $\exp\,(-\omega^2\pi^2 D_L t)$, which depends on its frequency.

The exact solution of the finite difference equation (3-10) is

$$C_{i,n} = \sum_{\omega=1}^{I-1} A_\omega \rho^n \sin \omega\pi(i\Delta x - u\phi n\Delta t) \qquad (3\text{-}13)$$

where the decay factor ρ and the velocity factor ϕ are each functions of $u\Delta t/\Delta x$, $D_L\Delta t/(\Delta x)^2$, $\omega\pi\Delta x$ and the weighting coefficients a_1 to b_3.

For the solution of the finite difference equation to approximate the exact solution, equation (3-12), for all frequencies ω and for any value of the dispersion coefficient, it is required that ρ approach unity as D_L approaches zero (no decay), and that ϕ be equal to 1 for all frequencies ω. Stone and Brian obtained the expressions for ρ and ϕ and determined the values of the weighting coefficients to meet these criteria. It was found that for ρ to approach unity when D_L approaches zero the conditions are

$$a_3 = a_2$$

$$a_4 = a_1 \qquad (3\text{-}14)$$

and $$b_3 = b_2$$

With these conditions the expression for ϕ has two degrees of freedom, given by a_2 and b_2. As $u\Delta t/\Delta x$ approaches zero the value of ϕ is determined by b_2 alone. It is not possible to make ϕ equal to unity for all values of the frequency ω. Their approach is to make ϕ as close to unity as possible for the low frequencies so that they are propagated at the correct velocity. The high frequencies will then travel at incorrect velocities. The decay factor decreases rapidly with increase in frequency (i.e. higher harmonics are decayed faster). The authors' suggestion is thus to include a minimal value of D_L, even when there is no dispersion, and thus to decay out the high harmonics. Although these harmonics travel with incorrect velocities they will be decayed so fast that they do not appear in the solution.

Taking the limit of ϕ as $u\Delta t/\Delta x$ approaches zero one gets a series expansion in $(\omega\pi\Delta x)$. The value of ϕ in the limit can be made unity for the fundamental frequency by setting $b_2 = 1/6$. An alternative method is to use equation (3-9) N times in each time step. Each time it is used a different value of b_2 is chosen. These values are chosen so that the arithmetic mean of the N values of ϕ in each time step is equal to unity. For $N = 3$ the results are $(b_2)_1 = 0.06250$, $(b_2)_2 = 0.20725$ and $(b_2)_3 = 0.23025$.

The value of a_2 is chosen as 0.25, which makes $a_1 = a_2 = a_3 = a_4 = 0.25$. This choice is made to have ϕ vary only slowly as $u\Delta t/\Delta x$ increases from zero.

Some results are presented in the paper for the case $D_L = 0$. They show an improvement over the results of all other schemes previously suggested.

It should be noted that the greatest difficulty arises from the singular case $D_L = 0$. The present work is not concerned with the behaviour of the finite difference equation for this special case. Only situations in which the dispersion coefficient has a finite value will be considered. In units of (cm) and (sec) the order of magnitude is usually $D_L = [0(10^{-2})$ to $0(10^{-1})]u$. If only this range is considered, the minimum value recommended by Stone and Brian for D_L is always available.

The next section describes a method used in the numerical solution of multi-dimensional heat conduction problems, which is another ingredient in the proposed numerical scheme.

3.3 The Alternating-Direction Method

Consider the two dimensional diffusion problem given by

$$\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} = \frac{\partial C}{\partial t} \tag{3-15}$$

where the variables have been transformed so that no coefficients appear in the equation. Let the equation describe the concentration distribution in the rectangle $0 \le x \le \ell x$, $0 \le y \le \ell y$, in which there exists some initial concentration distribution $C(x,y,0)$. Let $C_{i,j,n}$ denote the concentration at the point $x = i\Delta x$, $y = j\Delta y$ at time level n. Using the notation of equation (3-9) the explicit finite difference analogue of equation (3-15) is

$$\Delta_x^2\ (C_n) + \Delta_y^2\ (C_n) = \frac{C_{i,j,n+1} - C_{i,j,n}}{\Delta t} \tag{3-16}$$

This solution is stable subject to the restriction

$$\frac{\Delta t}{(\Delta x)^2} + \frac{\Delta t}{(\Delta y)^2} \le \frac{1}{2} \tag{3-17}$$

The solution of equation (3-16) is simple, but a large amount of computer time is needed to compute it.

An implicit scheme is given by

$$\Delta_x^2\ (C_{n+1}) + \Delta_y^2\ (C_{n+1}) = \frac{C_{i,j,n+1} - C_{i,j,n}}{\Delta t} \tag{3-18}$$

This scheme is unconditionally stable, i.e. there is no restriction on the time step. At each time level one has to solve a set of simultaneous equations, each involving the five unknowns $C_{i,j,n+1}$, $C_{i-1,j,n+1}$, $C_{i+1,j,n+1}$, $C_{i,j-1,n+1}$ and $C_{i,j+1,n+1}$. In the coefficient matrix which represents this set of simultaneous equations there is a diagonal term (corresponding to $C_{i,j,n+1}$), two adjacent terms, and two terms at some distance from the diagonal. At each time level this matrix has to be solved for the values of C_{n+1} at all points. Solutions of these matrices are obtained either by matrix inversion or some iterative technique.

In 1955 Peaceman and Rachford [82] proposed an unconditionally stable method for the solution of two-dimensional heat conduction problems which reduces the computational effort, compared to both the explicit and implicit techniques. The method is to solve two equations per time step.

In each equation one of the derivatives appears in explicit form, while the other is implicit. The alternating-direction equations are

$$\Delta_x^2 (C_{n+1/2}) + \Delta_y^2 (C_n) = \frac{C_{i,j,n+1/2} - C_{i,j,n}}{(\Delta t/2)} \tag{3-19}$$

$$\Delta_x^2 (C_{n+1/2}) + \Delta_y^2 (C_{n+1}) = \frac{C_{i,j,n+1} - C_{i,j,n+1/2}}{(\Delta t/2)} \tag{3-20}$$

Although each step is subject to a stability criterion, Peaceman and Rachford have shown that the combination of the two steps is unconditionally stable. The values of $C_{n+1/2}$ are therefore considered only as intermediate values, and are not used. For each time level one has to solve twice a tridiagonal set of equations. This turns out to be much less time consuming than a single solution of a matrix resulting from a full implicit scheme, by any of the known techniques.

For a mesh of (N x N) points the alternating direction method requires about $9N^2$ operation per time step. The implicit scheme, using the most efficient technique for the solution, requires at least $35N^2$ operations per time step. For a simple example presented in the paper the explicit scheme took 25 times as much work as the alternating direction scheme, and the implicit scheme 4 times as much.

Other alternating direction schemes have been proposed. Brian [67] suggested a scheme for three dimensional heat conduction problems. For the concentration diffusion problem in three-dimensions his scheme is given by the equations

$$\Delta_x^2 (C^*_{n+1/2}) + \Delta_y^2 (C_n) + \Delta_z^2 (C_n) = \frac{C^*_{i,j,k,n+1/2} - C_{i,j,k,n}}{(\Delta t/2)} \tag{3-21}$$

$$\Delta_x^2 (C^*_{n+1/2}) + \Delta_y^2 (C^{**}_{n+1/2}) + \Delta_z^2 (C_n)$$

$$= \frac{C^{**}_{i,j,k,n+1/2} - C_{i,j,k,n}}{(\Delta t/2)} \qquad (3\text{-}22)$$

$$\Delta_x^2 (C^*_{n+1/2}) + \Delta_y^2 (C^{**}_{n+1/2}) + \Delta_z^2 (C^{***}_{n+1/2})$$

$$= \frac{C^{***}_{i,j,k,n+1/2} - C_{i,j,k,n}}{(\Delta t/2)} \qquad (3\text{-}23)$$

$$\Delta_x^2 (C^*_{n+1/2}) + \Delta_y^2 (C^{**}_{n+1/2}) + \Delta_z^2 (C^{***}_{n+1/2})$$

$$= \frac{C_{i,j,k,n+1} - C_{i,j,k,n}}{\Delta t} \qquad (3\text{-}24)$$

The scheme is unconditionally stable and of high order accuracy. $C^*_{n+1/2}$, $C^{**}_{n+1/2}$ and $C^{***}_{n+1/2}$ denote successive approximations to $C_{n+1/2}$. Note that $C^*_{n+1/2}$ is used in the x-derivative in all equations, rather than the most recent approximation obtained. The same applies to the other derivatives. This results in an unconditionally stable scheme, as discussed by Brian in his paper [67].

3.4 The Proposed Numerical Scheme

The problem to be solved is the dispersion in a steady, three dimensional potential flow field in porous media, in which the miscible fluids have the same density and viscosity. The proposed numerical technique will be developed and tested for two dimensional flow fields. The extention to three dimensions is presented, and although it was not tested it is quite clear that the method is applicable in this case as well.

The proposed scheme seeks to take advantage of the Stone and Brian scheme, which was devised for the one dimensional case. For this reason the dispersion equation is used in Φ - ψ coordinates, equation (2-7). As the velocity is tangent to the lines of ψ = constant there is only one convective term in the equation, whereas the equation for two dimensional convective dispersion in Cartesian coordinates has in general a convective term in each of the coordinate directions. Further consequences of using this form of the equation, rather than the Cartesian form, will be discussed after the scheme has been presented.

Equation (2-7) may be put in a non dimensional form, using a reference length ℓ_0 and a reference velocity u_0 to define the non-dimensional variables

$$\eta = \frac{\Phi}{u_0 \ell_0} \qquad \xi = \frac{\psi}{u_0 \ell_0}$$

$$\tau = \frac{t\,u_0}{\ell_0} \qquad v = \frac{q}{u_0} \tag{3-25}$$

$$\alpha_L' = \frac{\alpha_L}{\ell_0} \qquad \alpha_T' = \frac{\alpha_T}{\ell_0} \qquad D_m' = \frac{D_m}{u_0 \ell_0}$$

With these variables equation (2-7) becomes

$$\frac{1}{v^2}\frac{\partial C}{\partial \tau} + \frac{\partial C}{\partial \eta} = \frac{\partial}{\partial \eta}\left[(\alpha_L' v + D_m')\frac{\partial C}{\partial \eta}\right] + \frac{\partial}{\partial \xi}\left[(\alpha_T' v + D_m')\frac{\partial C}{\partial \xi}\right] \tag{3-26}$$

C is a relative concentration, and therefore non-dimensional.

It is important to note that the coefficient (v^{-2}) in front of the time derivative arises from the basic consideration of continuity in the curvilinear Φ - ψ coordinate system, and not from the expansion of a derivative (see Hoopes and Harleman, p. 64). It is advisable to use the differential equation in its most basic form, where one can identify physical fluxes of mass. The finite difference analogue should include differences between fluxes, rather than simply replace derivatives by their finite difference approximation. Thus one should not expand the right hand side of equation (3-26) because one replaces fluxes of mass by spatial variations of concentration gradients and velocities.

The proposed finite difference analogue of equation (3-26) is given by the following set of equations:

$$- \left[DL_{i+1/2} \frac{(C^*_{i+1,j,n+1} - C^*_{i,j,n+1})}{(\Delta\eta)^2} - DL_{i-1/2} \frac{(C^*_{i,j,n+1} - C^*_{i-1,j,n+1})}{(\Delta\eta)^2} \right]$$

$$- \left[DT_{j+1/2} \frac{(C_{i,j+1,n} - C_{i,j,n})}{(\Delta\xi)^2} - DT_{j-1/2} \frac{(C_{i,j,n} - C_{i,j-1,n})}{(\Delta\xi)^2} \right]$$

$$+ \frac{1}{\Delta\eta} \Big[a_1(C_{i+1,j,n} - C_{i,j,n}) + a_2(C_{i,j,n} - C_{i-1,j,n})$$

$$+ a_3(C^*_{i+1,j,n+1} - C^*_{i,j,n+1}) + a_4(C^*_{i,j,n+1} - C^*_{i-1,j,n+1}) \Big]$$

$$+ \frac{1}{v^2_{i,j}\Delta\tau} \Big[b_1(C^*_{i,j,n+1} - C_{i,j,n}) + b_2(C^*_{i+1,j,n+1} - C_{i+1,j,n})$$

$$+ b_3(C^*_{i-1,j,n+1} - C_{i-1,j,n}) \Big] = 0 \qquad (3\text{-}27)$$

$$- \left[DL_{i+1/2} \frac{(C^*_{i+1,j,n+1} - C^*_{i,j,n+1})}{(\Delta\eta)^2} - DL_{i-1/2} \frac{(C^*_{i,j,n+1} - C^*_{i-1,j,n+1})}{(\Delta\eta)^2} \right]$$

$$- \left[DT_{j+1/2} \frac{(C^{**}_{i,j+1,n+1} - C^{**}_{i,j,n+1})}{(\Delta\xi)^2} - DT_{j-1/2} \frac{(C^{**}_{i,j,n+1} - C^{**}_{i,j-1,n+1})}{(\Delta\xi)^2} \right]$$

$$+ \frac{1}{\Delta\eta} \Big[a_1(C_{i+1,j,n} - C_{i,j,n}) + a_2(C_{i,j,n} - C_{i-1,j,n})$$

$$+ a_3(C^*_{i+1,j,n+1} - C^*_{i,j,n+1}) + a_4(C^*_{i,j,n+1} - C^*_{i-1,j,n+1}) \Big]$$

$$+ \frac{1}{v^2_{i,j}\Delta\tau} \Big[b_1(C^{**}_{i,j,n+1} - C_{i,j,n}) + b_2(C^*_{i+1,j,n+1} - C_{i+1,j,n})$$

$$+ b_3(C^*_{i-1,j,n+1} - C_{i-1,j,n}) \Big] = 0 \qquad (3\text{-}28)$$

and

$$-\left[DL_{i+1/2}\,\frac{(C^{*}_{i+1,j,n+1}-C^{*}_{i,j,n+1})}{(\Delta\eta)^{2}}-DL_{i-1/2}\,\frac{(C^{*}_{i,j,n+1}-C^{*}_{i-1,j,n+1})}{(\Delta\eta)^{2}}\right]$$

$$-\left[DT_{j+1/2}\,\frac{(C^{**}_{i,j+1,n+1}-C^{**}_{i,j,n+1})}{(\Delta\xi)^{2}}-DT_{j-1/2}\,\frac{(C^{**}_{i,j,n+1}-C^{**}_{i,j-1,n+1})}{(\Delta\xi)^{2}}\right]$$

$$+\frac{1}{\Delta\eta}\Big[a_1(C_{i+1,j,n}-C_{i,j,n})+a_2(C_{i,j,n}-C_{i-1,j,n})$$

$$+a_3(C^{*}_{i+1,j,n+1}-C^{*}_{i,j,n+1})+a_4(C^{*}_{i,j,n+1}-C^{*}_{i-1,j,n+1})\Big]$$

$$+\frac{1}{v^{2}_{i,j}\Delta\tau}\left[C_{i,j,n+1}-C_{i,j,n}\right]=0 \qquad (3\text{-}29)$$

where

$$DL_{i+1/2}=\frac{(\alpha'_L\,v_{i+1,j}+D'_m)+(\alpha'_L\,v_{i,j}+D'_m)}{2} \qquad (3\text{-}30)$$

$$DL_{i-1/2}=\frac{(\alpha'_L\,v_{i,j}+D'_m)+(\alpha'_L\,v_{i-1,j}+D'_m)}{2} \qquad (3\text{-}31)$$

$$DT_{j+1/2}=\frac{(\alpha'_T\,v_{i,j+1}+D'_m)+(\alpha'_T\,v_{i,j}+D'_m)}{2} \qquad (3\text{-}32)$$

and

$$DT_{j-1/2}=\frac{(\alpha'_T\,v_{i,j}+D'_m)+(\alpha'_T\,v_{i,j-1}+D'_m)}{2} \qquad (3\text{-}33)$$

Equation (3-27) is solved for C^{*}_{n+1}. Then C_n and C^{*}_{n+1} are used in equation (3-28) to solve for C^{**}_{n+1}. Both C^{*}_{n+1} and C^{**}_{n+1} are intermediate values which are then used in equation (3-29) to solve for C_{n+1}. Before discussing these equations it will be convenient to put them in the following symbolic form

EQ	STEP	Δ_η	Δ^2_η	Δ^2_ξ	Δ_τ
3-27	$\Delta\tau$	(n) & $(n+1)^*$ WEIGHTED	$(n+1)^*$	(n)	$[(n+1)^* - (n)]$ WEIGHTED
3-28	—"—	—"—	—"—	$(n+1)^{**}$	$[(n+1)^{**} - (n)]$ $[(n+1)^* - (n)]$ WEIGHTED
3-29	—"—	—"—	—"—	—"—	$[(n+1) - (n)]$

The motivation for using the convective dispersion equation in $\Phi - \psi$ coordinates was to be able to devise a numerical scheme which makes use of Stone and Brian's results for the one dimensional case, while keeping the scheme efficient by using the alternating direction method. Stone and Brian's weighting scheme for the convective and time terms is used without modification. The magnitude of the weighting coefficients is the same even though the convective term in equation (2-7) is non-linear, whereas the scheme was developed for the linear equation. This can be done because of another property of the equation in $\Phi - \psi$ coordinates. In a homogeneous isotropic medium one can write

$$q \cong \frac{\Delta\Phi}{\Delta S_\Phi}$$

where ΔS_Φ is the physical distance along the streamline between adjacent equipotentials. Then, if $\Delta\Phi$ = const

$$q \cdot \Delta S_\Phi \cong \text{const}$$

This relation implies that the velocity at adjacent grid points has equal "weighting" on either side of the grid point under consideration. If the convective dispersion equation had been used in Cartesian coordinates, not only would it include in general two convective terms, but the weighting scheme would depend on the local pattern of spatial variation of the velocity.

Another motivation for the proposed scheme was the hope that the dispersion at right angles to the direction of the velocity could be treated with a technique applicable to diffusion problems, namely the alternating direction method. The effect of lateral dispersion is secondary while the convection has a dominating effect on the solution. If the convective term is treated correctly, the superposition of longitudinal and lateral dispersion on the convective solution should yield correct results.

The proposed method achieves an increase in efficiency over both the explicit and implicit schemes, as will be demonstrated in Chapter IV. The price paid is a more complicated programming task, but this promises to be a one-time effort which yields general results. The additional programming needed to solve any particular problem will be minimal.

As the scheme is unconditionally stable the time step is not restricted in magnitude. The convergence of the numerical solution to the true solution does depend, however, on the magnitude of the time step. The time step has to be small when there exist large spatial gradients in the concentration distribution. In the presence of a step in concentration, for example, the initial time step should be chosen so the front travels one space increment in several time steps. The time step may be increased as the sharp front is dispersed.

The efficiency of the scheme is strongly dependent on the sequence of time steps used in the computations. Although there is no theoretical means of predicting the optimal sequence to achieve accuracy with a minimum of computer time, some guidelines based on experience will be given in sections dealing with results. Each example will be accompanied by the time step sequence used in the computation. The sequence is determined by assigning an initial (minimum) value to $\Delta\tau/\Delta\eta$, multiplying $\Delta\tau$ by a constant factor at each time level, until a maximum value of $\Delta\tau/\Delta\eta$ has been reached. From that time on $\Delta\tau$ = constant.

One of the advantages of the proposed scheme is its generality. Equation (3-26) is applicable to any steady two dimensional potential flow field. The geometry of the flow field enters through the expression for the seepage velocity $v = v(\eta,\xi)$. The flow field need not be described by an analytical expression for the seepage velocity. The seepage velocity may be given as a table of values obtained from measurements. The equations for the streamlines and equipotentials in any potential flow field may be obtained from measurements of the potential at points in the field. Nelson [38] describes computer programs which were developed to perform such calculations.

Other schemes may be proposed which use the Stone and Brian scheme for the Φ-direction and an alternating direction scheme for dealing with the ψ-direction. One such method was tried but gave results which were not as good as those of the proposed scheme. Its symbolic representation is

EQ.	STEP	Δ_η	Δ^2_η	Δ^2_ξ	Δ_τ
1st	$\frac{\Delta\tau}{2}$	$(n)\&(n+1/2)^*$ WEIGHTED	$(n+1/2)^*$	(n)	$[(n+1/2)^* - (n)]$ WEIGHTED
2nd	$\frac{\Delta\tau}{2}$	—— " ——	—— " ——	$(n+1/2)^{**}$	$[(n+1/2)^{**} - (n)]$
3rd	$\Delta\tau$	—— " ——	—— " ——	—— " ——	$[(n+1) - (n)]$

In this scheme the intermediate values are computed at (n+1/2), and the time derivative in the 2nd equation is not weighted and is just

$$\frac{1}{v^2_{i,j}\Delta\tau}\left[C^{**}_{i,j,n+1/2} - C_{i,j,n}\right]$$

The formulation of the proposed numerical scheme provides a great flexibility in its use. One may use the first equation as a complete numerical scheme for cases in which $\alpha_T = 0$, or when there exist no lateral concentration gradients. Equation (3-27) describes convection and dispersion along a streamline, and there is no influence of the concentration on adjacent streamlines. This scheme can also be used to get approximate answers in cases where lateral concentration exists, but the lateral dispersion term is small. From data reported in the literature α_T is in the range of $(0.05 \text{ to } 0.1)\alpha_L$, and unless the lateral concentration distribution has a strong curvature the lateral dispersion term can be neglected as compared with the other terms in the equation. The use of this abbreviated scheme provides a substantial saving in computer time compared to the full scheme.

If lateral dispersion is taken into consideration, but has little effect, one may use a second abbreviated scheme. The scheme then includes equations (3-27) and (3-28), and the values of C^{**} computed from equation (3-28) are taken as C_{n+1}, the new concentration.

The option of using equation (3-27) only, the first two equations or the full three equation scheme was included in the computer program. The scheme selected is specified with the input data. Considerable economy in computer time may be achieved by judicious use of the abbreviated schemes.

The extension of the proposed scheme to include three dimensional problems is obvious. There still is only one convective term, and the lateral dispersion (this time in two directions perpendicular to the streamline) can be dealt with by the alternating direction method. The convective dispersion in $\Phi - \psi_1 - \psi_2$ coordinates for a three dimensional steady potential flow field is

$$\begin{aligned}\frac{\partial C}{\partial t} + q^2 \frac{\partial C}{\partial \Phi} = q^2 \frac{\partial}{\partial \Phi}&\left[(\alpha_L q + D_m) \frac{\partial C}{\partial \Phi}\right] \\ &+ q^2 \frac{\partial}{\partial \psi_1}\left[(\alpha_T q + D_m) \frac{\partial C}{\partial \psi_1}\right] \\ &+ q^2 \frac{\partial}{\partial \psi_2}\left[(\alpha_T q + D_m) \frac{\partial C}{\partial \psi_2}\right] \qquad (3\text{-}34)\end{aligned}$$

The formulation of the proposed numerical scheme provides a great flexibility in its use. One may use the first equation as a complete numerical scheme for cases in which $\alpha_T = 0$, or when there exist no lateral concentration gradients. Equation (3-27) describes convection and dispersion along a streamline, and there is no influence of the concentration on adjacent streamlines. This scheme can also be used to get approximate answers in cases where lateral concentration exists, but the lateral dispersion term is small. From data reported in the literature α_T is in the range of $(0.05 \text{ to } 0.1)\alpha_L$, and unless the lateral concentration distribution has a strong curvature the lateral dispersion term can be neglected as compared with the other terms in the equation. The use of this abbreviated scheme provides a substantial saving in computer time compared to the full scheme.

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$$\begin{aligned}\frac{\partial C}{\partial t} + q^2 \frac{\partial C}{\partial \Phi} = q^2 \frac{\partial}{\partial \Phi}\left[(\alpha_L q + D_m)\frac{\partial C}{\partial \Phi}\right] \\ + q^2 \frac{\partial}{\partial \psi_1}\left[(\alpha_T q + D_m)\frac{\partial C}{\partial \psi_1}\right] \\ + q^2 \frac{\partial}{\partial \psi_2}\left[(\alpha_T q + D_m)\frac{\partial C}{\partial \psi_2}\right] \qquad (3\text{-}34)\end{aligned}$$

where Φ = constant are the equipotential surfaces, ψ_1 = constant and ψ_2 = constant are two families of orthogonal stream surfaces.

The numerical scheme for the solution of equation (3-34) is presented only in the symbolic form

EQ.	STEP	$\Delta\eta$	Δ^2_η	$\Delta^2_{\xi_1}$	$\Delta^2_{\xi_2}$	$\Delta\tau$
1st	$\Delta\tau$	(n) & $(n+1)^*$ WEIGHTED	$(n+1)^*$	(n)	(n)	$[(n+1)^* - (n)]$ WEIGHTED
2nd	—"—	——"——	—"—	$(n+1)^{**}$	—"—	$[(n+1)^{**} - (n)]$& $[(n+1)^* - (n)]$ WEIGHTED
3rd	—"—	——"——	—"—	—"—	$(n+1)^{***}$	$[(n+1)^{***} - (n)]$& $[(n+1)^* - (n)]$ WEIGHTED
4th	—"—	——"——	—"—	—"—	—"—	$[(n+1) - (n)]$

The 1st, 2nd and 4th equations are similar to equations (3-27) to (3-29), except that they include $\Delta^2_{\xi_2}(C_n)$ or $\Delta^2_{\xi_2}(C^{***}_{n+1})$. The time term in the third equation is

$$\frac{1}{v^2_{i,j}\Delta\tau}\Big[b_1(C^{***}_{i,j,k,n+1} - C_{i,j,k,n}) + b_2(C^*_{i+1,j,k,n+1} - C_{i+1,j,k,n}) + b_3(C^*_{i-1,j,k,n+1} - C_{i-1,j,k,n})\Big] \qquad (3\text{-}35)$$

The proposed technique has been used for some cases of one-dimensional flow in non-homogeneous media. Results are presented in Chapter V. It is believed that the technique is also applicable to anisotropic media, although this has not been tried.

Possible extensions to other, more general, cases will be discussed in Chapter VI as suggestions for future work.

3.5 The Computational Scheme

For each time step the set of equations for the two-dimensional case includes two implicit equations and one explicit equation. Equation (3-27) is solved for $C^*_{i-1,j,n+1}$, $C^*_{i,j,n+1}$ and $C^*_{i+1,j,n+1}$. At each point the equation has the form

$$\zeta_\eta \, C^*_{i-1,j,n+1} + \beta_\eta \, C^*_{i,j,n+1} + \gamma_\eta \, C^*_{i+1,j,n+1} =$$

$$= \delta_1 \, C_{i-1,j,n} + \delta_2 \, C_{i,j,n} + \delta_3 \, C_{i+1,j,n} +$$

$$+ \delta_4 \, C_{i,j-1,n} + \delta_5 \, C_{i,j+1,n} \tag{3-36}$$

where the coefficients are given by

$$\zeta_\eta = \frac{b_3}{v^2_{i,j}\Delta\tau} - \frac{DL_{i-1/2}}{(\Delta\eta)^2} - \frac{a_4}{\Delta\eta}$$

$$\beta_\eta = \frac{b_1}{v^2_{i,j}\Delta\tau} + \frac{DL_{i-1/2} + DL_{i+1/2}}{(\Delta\eta)^2} + \frac{(a_4 - a_3)}{\Delta\eta}$$

$$\gamma_\eta = \frac{b_2}{v^2_{i,j}\Delta\tau} - \frac{DL_{i+1/2}}{(\Delta\eta)^2} + \frac{a_3}{\Delta\eta}$$

$$\delta_1 = \frac{b_3}{v^2_{i,j}\Delta\tau} + \frac{a_2}{\Delta\eta}$$

$$\delta_2 = \frac{b_1}{v^2_{i,j}\Delta\tau} - \frac{(DT_{j-1/2} + DT_{j+1/2})}{(\Delta\xi)^2} + \frac{(a_1 - a_2)}{\Delta\eta}$$

$$\delta_3 = \frac{b_2}{v^2_{i,j}\Delta\tau} - \frac{a_1}{\Delta\eta}$$

$$\delta_4 = \frac{DT_{j-1/2}}{(\Delta\xi)^2}$$

and $$\delta_5 = \frac{DT_{j+1/2}}{(\Delta\xi)^2}$$

For the second step equation (3-27) is subtracted from equation (3-28) to yield

$$- DT_{j+1/2} \frac{(C^{**}_{i,j+1,n+1} - C^{**}_{i,j,n+1}) - (C_{i,j+1,n} - C_{i,j,n})}{(\Delta\xi)^2}$$

$$+ DT_{j-1/2} \frac{(C^{**}_{i,j,n+1} - C^{**}_{i,j-1,n+1}) + (C_{i,j,n} - C_{i,j-1,n+1})}{(\Delta\xi)^2}$$

$$+ \frac{1}{v^2_{i,j}\Delta\tau} \left[b_1 (C^{**}_{i,j,n+1} - C^{*}_{i,j,n+1}) \right] = 0 \qquad (3\text{-}37)$$

This equation has the form

$$\zeta_\xi \, C^{**}_{i,j-1,n+1} + \beta_\xi \, C^{**}_{i,j,n+1} + \gamma_\xi \, C^{**}_{i,j+1,n+1} =$$

$$= \delta_6 \, C_{i,j-1,n} + \delta_7 \, C_{i,j,n} + \delta_8 \, C_{i,j+1,n} + \delta_9 \, C_{i-1,j,n} +$$

$$+ \delta_{10} \, C_{i+1,j,n} + \rho_1 \, C^{*}_{i,j,n+1} + \rho_2 \, C^{*}_{i+1,j,n+1} +$$

$$+ \rho_3 \, C^{*}_{i-1,j,n+1} \qquad (3\text{-}38)$$

where

$$\zeta_\xi = \frac{- DT_{j-1/2}}{(\Delta\xi)^2}$$

$$\beta_\xi = \frac{b_1}{v^2_{i,j}\Delta\tau} + \frac{DT_{j-1/2} + DT_{j+1/2}}{(\Delta\xi)^2}$$

$$\gamma_\xi = \frac{- DT_{j+1/2}}{(\Delta\xi)^2}$$

$$\delta_6 = \zeta_\xi = \frac{- DT_{j-1/2}}{(\Delta\xi)^2}$$

$$\delta_7 = \frac{DT_{j-1/2} + DT_{j+1/2}}{(\Delta\xi)^2}$$

$$\delta_8 = \gamma_\xi = \frac{-\,DT_{j+1/2}}{(\Delta\xi)^2}$$

and

$$\rho_1 = \frac{b_1}{v^2_{i,j}\Delta\tau}$$

$\delta_9 = \delta_{10} = \rho_2 = \rho_3 = 0$ were included in the general form, equation (3-38), because other finite difference analogues may be suggested, and in general C^{**}_{n+1} is a function of C_n at five points and C^{*}_{n+1} at three points.

The third step in the scheme is the explicit solution of equation (3-29) for $C_{i,j,n+1}$. The general form of the equation is

$$\begin{aligned} C_{i,j,n+1} &= P_1\, C_{i,j,n} + P_2\, C_{i-1,j,n} + P_3\, C_{i+1,j,n} \\ &\quad + Q_1\, C^{*}_{i-1,j,n+1} + Q_2\, C^{*}_{i,j,n+1} + Q_3\, C^{*}_{i+1,j,n+1} \\ &\quad + S_1\, C^{**}_{i,j-1,n+1} + S_2\, C^{**}_{i,j,n+1} + S_3\, C^{**}_{i,j+1,n+1} \end{aligned} \tag{3-39}$$

where

$$P_1 = 1 + \frac{(a_1 - a_2)\,\Delta\tau\, v^2_{i,j}}{\Delta\eta}$$

$$P_2 = \frac{a_2\, v^2_{i,j}\,\Delta\tau}{\Delta\eta}$$

$$P_3 = \frac{-\,a_1\, v^2_{i,j}\,\Delta\tau}{\Delta\eta}$$

$$Q_1 = \frac{DL_{i-1/2}\, v^2_{i,j}\,\Delta\tau}{(\Delta\eta)^2} + \frac{a_4\, v^2_{i,j}\,\Delta\tau}{\Delta\eta}$$

$$Q_2 = -\frac{(DL_{i-1/2} + DL_{i+1/2})v^2_{i,j}\,\Delta\tau}{(\Delta\eta)^2} + \frac{(a_3 - a_4)v^2_{i,j}\,\Delta\tau}{\Delta\eta}$$

$$Q_3 = \frac{DL_{i+1/2}\, v^2_{i,j}\,\Delta\tau}{(\Delta\eta)^2} - \frac{a_3\, v^2_{i,j}\,\Delta\tau}{\Delta\eta}$$

$$S_1 = \frac{DT_{j-1/2}\, v^2_{i,j}\, \Delta\tau}{(\Delta\xi)^2}$$

$$S_2 = -\frac{(DT_{j-1/2} + DT_{j+1/2}) v^2_{i,j}\, \Delta\tau}{(\Delta\xi)^2}$$

$$S_3 = \frac{DT_{j+1/2}\, v^2_{i,j}\, \Delta\tau}{(\Delta\xi)^2}$$

Equations (3-36) and (3-38) result in a tri-diagonal set of simultaneous equations. In forming the first and last equation of each set three possible types of boundary conditions were considered.

3.5.1 The Reflection Boundary Condition

A reflection condition at the boundary corresponds to the condition $\partial C/\partial n = 0$ at the boundary, where n is the direction normal to the boundary. It is achieved in the numerical solution by addition of a fictitious grid point outside the field at a distance from the boundary equal to the grid spacing, and setting the value of the concentration there equal to the concentration at the first point inside the field.

Thus a reflection condition at the boundary point C(1,j) corresponds to setting

$$C_{0,j} = C_{2,j}$$

which can be represented graphically as

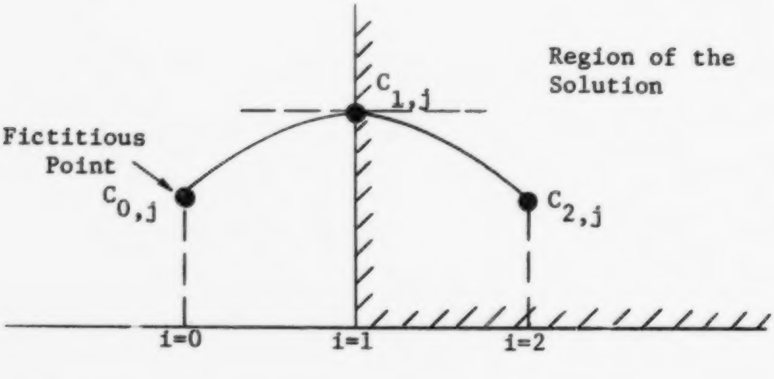


Fig. 3-4: The Reflection Boundary Condition

3.5.2 The Transmission Boundary Condition

This condition guarantees a continuation of the slope of the concentration distribution through the boundary. When applied at point (1,j) it gives

$$C_{0,j} = 2C_{1,j} - C_{2,j}$$

which may be seen from Fig. 3-5

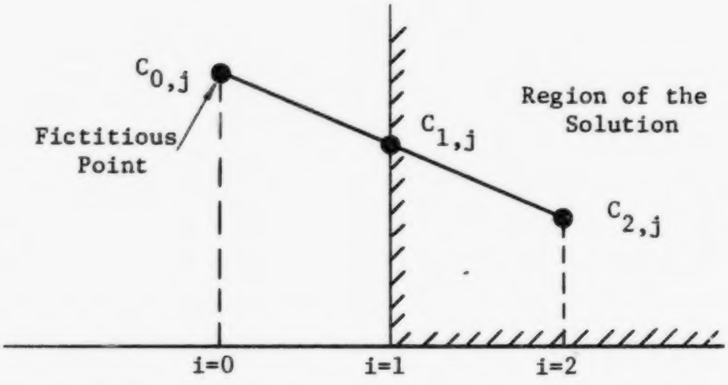


Fig. 3-5 The Transmission Boundary Condition

3.5.3 A Known Value

When the value at the boundary is either constant or a known function of time it may be transferred to the right hand side and included in Δ_1 or Δ_k (see Section 3.5.6).

3.5.4 The Initial Condition

It was decided to use in all examples the initial condition

$$C_{i,j,0} = 0 \qquad i = 1, \cdots, I \quad j = 1, \ldots, J$$

$$C_{1,j,n} = 1 \qquad j_{min} \le j \le j_{max}, \text{ all } n$$

This corresponds to a step function in the input concentration along some portion of the inflow boundary i = 1. The flow is in the direction of increasing η because of the definition of the velocity as

$$q = \frac{d\Phi}{ds}$$

so the inflow boundary is $\eta = \eta_{min}$.

There were two reasons for using this initial and boundary conditions:

a. Harmonics of all frequencies are present in the step function, so this poses the most difficult situation with respect to accuracy and efficiency (time step sequence).

b. This is a condition often encountered in field situations.

A few cases were tried with initial conditions which were smooth functions of space or time, and it was found that the initial time steps could be taken larger, and could be increased faster than in the case of a step input in concentration without loss of accuracy.

3.5.5 The Time-Step Sequence

The parameter $u\Delta t/\Delta x$, which governs the accuracy of the solution in the one-dimensional case, has the same value at any point in the flow field because u = const. In the general case of two-dimensional flow q varies from point to point. The non dimensional form of this parameter is

$$\frac{q\ \Delta t}{\Delta\Phi} = \left(\frac{v}{u_0}\right) \frac{\Delta\tau}{\Delta\eta} \tag{3-40}$$

so $\Delta\tau/\Delta\eta$ may be used as the criterion. u_0 has to be chosen such that v/u_0 is approximately unity in the region where a step occurs. If this is done the experience gained from studying the optimal time-step sequence for the one dimensional case may be applied to other cases.

3.5.6 The Thomas Algorithm

The numerical solution requires to solve tri-diagonal matrices. The large number of times such a solution is needed makes the method by which it is obtained, a very important factor in the efficiency and accuracy of the scheme. This section outlines the algorithm which has been used.

The set of K simultaneous equations given by

$$\zeta_k C_{k-1} + \beta_k C_k + \gamma_k C_{k+1} = \Delta_k, \quad k = 1, \cdots, K \qquad (3\text{-}41)$$

may be represented in matrix form

$$\begin{bmatrix} \beta_1 & \gamma_1' & & & & & & \\ \zeta_2 & \beta_2 & \gamma_2 & & & & & \\ & \zeta_3 & \beta_3 & \gamma_3 & & & & \\ & & \text{—} & \text{—} & \text{—} & & & \\ & & & \zeta_k & \beta_k & \gamma_k & & \\ & & & & \text{—} & \text{—} & \text{—} & \\ & & & & & \zeta_{K-1} & \beta_{K-1} & \gamma_{K-1} \\ & & & & & & \zeta_K' & \beta_K \end{bmatrix} \cdot \begin{bmatrix} \\ C_k \\ \\ \end{bmatrix} = \begin{bmatrix} \\ \Delta_k \\ \\ \end{bmatrix}$$

where the primes on γ_1' and ζ_K' denote that these coefficients have been computed from the boundary conditions described in the previous sections (e.g. for reflection at $k = 1$ $\gamma_1' = \zeta_1 + \gamma_1$).

The solution proceeds as follows:

a. Combine the 1st and 2nd equations to eliminate ζ_2. The new form of the second equation is

$$V_2 C_2 + \gamma_2 C_3 = W_2 \qquad (3\text{-}42)$$

store the values V_2 and W_2, and

b. Combine equation (3-42) with the 3rd equation to eliminate ζ_3, and get

$$V_3 C_3 + \gamma_3 C_4 = W_3 \qquad (3\text{-}43)$$

c. Proceed to the following equations, storing the values of V_k and W_k given by

$$V_k = \beta_k - \frac{\zeta_k}{V_{k-1}} \gamma_{k-1} \qquad k = 2,\cdots, K \qquad (3\text{-}44)$$

and

$$W_k = \Delta_k - \frac{\zeta_k}{V_{k-1}} W_{k-1} \qquad k = 2,\cdots, K \qquad (3\text{-}45)$$

with

$V_1 = \beta_1$ and $W_1 = \Delta_1$

d. Solve for C_K from the last equation

$$C_K = \frac{W_K}{V_K}$$

e. Solve in reversed order for

$$C_k = \frac{W_k - \gamma_k C_{k+1}}{V_k} \qquad k = K-1,\cdots, 1 \qquad (3\text{-}46)$$

The storage needed for the computations (in addition to the arrays C, C^* and C^{**}) is twice the number of rows of the matrix, provided ζ, β, γ and the δ's are calculated for a point whenever needed, and are not saved in storage.

3.6 General Description of the Computer Program

The computational scheme was programmed in FORTRAN II for the IBM 7094 Computer at the M.I.T. Computation Center. Flow charts and listings are included in Appendix A along with definitions of the symbols used and instructions for the user.

The MAIN program accepts the input data and computes the non-dimensional quantities. It governs the sequence of operations to be performed, after having selected the scheme option (one, two or three equations). The tri-diagonal matrix resulting from equation (3-27) is solved in SUBROUTINE TDETA (Tri-Diagonal for the ETA equation). It solves for C^* using the known values of C. The tri-diagonal matrix resulting from equation (3-28) is solved for C^{**}, using the known values of C and C^*, in SUBROUTINE TDCSI. It was convenient to solve for each direction in a separate subroutine, rather than write a general tri-diagonal solving routine. The explicit solution for C_{n+1}, equation (3-29), is performed by SUBROUTINE EXPLIC.

The coefficients for these subroutines are given in separate subroutines. Thus SUBROUTINE C4ETA(I,J) (Coefficients FOR ETA) computes ζ_η, β_η, γ_η and δ_1 to δ_5 at the point (I,J). C4CSI(I,J) and CFEXP(I,J) give the coefficients for TDCSI and EXPLIC, respectively.

The coefficients are given in separate subroutines because they depend on the specific problem solved, through the expression for $v_{i,j}$. Thus these subroutines are unique to the problem, and have to be re-written for each problem. It is, however, only the expression for $v_{i,j} = (i\Delta\eta, j\Delta\xi)$ which has to be re-written, the rest of these coefficient subroutines is still valid.

Other general service subroutines are:

SUBROUTINE CINPUT sets the given boundary condition for the concentration along the inflow equipotential ($\eta = \eta_{min}$).

SUBROUTINE USPRNT is a printout subroutine.

SUBROUTINE USMAP provides a graphical output on the high speed printer. Letters and symbols of different light density are used to express values of concentrations. 45 light-density levels were used, as may be seen in the subroutine. These correspond to concentration in the ranges 0 to 1/45, 1/45 to 2/45, · · · ·, 44/45 to 1.0. When used, this "MAP" enables one to see the shape of the concentration distribution in the whole field at a glance.

IV. DISPERSION IN HOMOGENEOUS-ISOTROPIC POROUS MEDIA

The purpose of this chapter is to bear out the statements made in Chapter III about the properties of the proposed numerical scheme, and at the same time present some results which have not been obtained before. The properties examined are:

a. Accuracy

To determine the accuracy of the proposed scheme it was applied to the problem of longitudinal dispersion in unidirectional flow. The results are compared with the analytical solution. The computation time needed to compute the solution is small, therefore many runs could be made to determine the effect of different parameters on the accuracy. Numerical solutions for more complex problems are compared with approximate analytical solutions obtained by others.

The accuracy of the numerical solution for the one-dimensional case is examined as a function of the relative magnitude of the coefficients in the differential equation, and of the time step sequence. This last factor also affects the efficiency.

b. Efficiency

The efficiency of the scheme is measured by the computation time required to obtain the solution to a problem with some predetermined degree of accuracy. The efficiency may be improved by a proper choice of the time step sequence and the number of cycles used. The results obtained for the one-dimensional case are helpful in determining the optimal combination to be used in more general cases. The efficiency of the scheme in solving more general two-dimensional problems can be evaluated by comparing the computation time used in this work with that required by other investigators to obtain numerical solutions to the same problem. This information is available only for the cases of radial flow and the two-well problem.

c. Generality and Flexibility of the Scheme and the Computer Program

It was stated that the scheme is applicable to any problem of dispersion in a steady two-dimensional flow field, and that the computer program requires only minor additions to apply it to any specific problem.

Although special programs were written for the one-dimensional problem and for radial flow, the same results could be obtained from the general program 2F2D. The purpose of these special programs was merely to allow more flexibility in their use.

The two-dimensional program was used for the problem of longitudinal and lateral dispersion in uni-directional flow, and for the two-well problem. The subroutines used to compute the coefficients for both these cases are presented in Appendix A. The subroutines vary from one case to the other only in the expression for the dimensionless seepage velocity $v(\eta,\xi)$. For any other steady two-dimensional flow field only the expression for $V(\eta,\xi)$ will have to be changed.

The existing program allows only two types of input concentration: a step over the whole inflow section, and a step over a part of the inflow section. Other types of input may be added in SUBROUTINE CINPUT.

The program allows only one initial condition, that of zero concentration throughout the flow field for $t \leq 0$. Setting this condition is done in the MAIN program. If other initial conditions are desired this may easily be incorporated into the program, in the MAIN or in a subroutine.

4.1 Longitudinal Dispersion in Steady Uni-Directional Flow

It has been stated in Chapter III that the most important part in the numerical scheme is the treatment of convection and dispersion in the direction of the flow. Much can be learned about the behaviour of the solutions for two-dimensional flow fields by examining the one-dimensional case. This amounts to programming Stone and Brian's scheme, as presented in their paper.

There is an exact analytical solution to the one dimensional problem for any type of input concentration, in particular for the step input considered in this work. Stone and Brian give in their paper only a few results, and focus on the case $D_L = 0$.

It is the purpose of this work to devise a tool for the solution of practical problems. For this reason the case $D_L = 0$ was not considered typical. It is interesting to examine the behaviour of the numerical solution for this case, but more emphasis is put on cases where

$$D_L\ (\text{cm}^2/\text{sec}) = [0(10^{-2})\ \text{to}\ 0(10^{-1})]\cdot[u(\text{cm/sec})] \qquad (4\text{-}1)$$

which is the range found in experiments.

The accuracy of the solution is improved with an increase in the value of the dispersion coefficient. This is due to the fact that the sharp front is dispersed more rapidly and the longitudinal concentration gradients are reduced.

If equation (4-1) is taken as the range of values encountered in actual problems, it is usually the value of the parameter $(u\Delta t/\Delta x)$ which determines the accuracy of the solution. If D_L is increased much beyond this range, the parameter $D_L\Delta t/(\Delta x)^2$ may become important, and its magnitude will determine the accuracy of the solution.

A computer program named 1F1D (1-dimensional Flow with 1-dimensional Dispersion) was written especially for this case. The general program, 2F2D, was not used because for the one dimensional case one needs only single-subscripted arrays (for C_i and C_i^*), which permits the use of a larger number of grid points without exceeding the capacity of the computer memory. There is need in one subroutine only for solving a tri-diagonal matrix. The tri-diagonal equations to be solved are of the form

$$\zeta C^*_{i-1,n+1} + \beta C^*_{i,n+1} + \gamma C^*_{i+1,n+1} = \delta_1 C_{i-1,n} + \delta_2 C_{i,n} + \\ + \delta_3 C_{i+1,n} \qquad (4\text{-}2)$$

SUBROUTINE TD1DIM, used to solve the equations given by (4-2), is simpler than TDETA because it uses only 3 known values to compute the right hand side. SUBROUTINE TD1DIM calls for calculating the coefficients ζ, β, γ and δ's for each grid point at each time level, rather than only once per time level for all points. For a homogeneous medium this represents a great waste of computer time, as the coefficient subroutine, C4TD1D(I), has to be called twice per time level for each point. There are two reasons for doing this:

a. The program is more general and can handle non-homogeneous media, in which the coefficients are functions of space, and

b. From the length of time it takes to solve the one-dimensional problem, with a certain number of grid points, one may infer the length of time it takes to solve the first equation of the two-dimensional scheme with the same number of grid points along a streamline.

The one dimensional program was used to gain some experience about the effect of the relative magnitude of the coefficients in the differential equation on the accuracy of the solution. At the same time the efficiency of the scheme, expressed as the amount of computer time required to compute the solution, was examined. The results of 11 runs are presented, and then discussed. The data for these runs are given in Table 4-1, and the results presented in Figures 4-1 through 4-11. All runs used the step input in concentration at $x = 0$, and a reflection boundary condition (corresponding to $\partial C/\partial x = 0$) at $x = \ell_x$. The exact analytical solution for this case is

$$\frac{C}{C_0} = \frac{1}{2} \operatorname{erfc} \left[\frac{x - ut}{2\sqrt{D_L t}}\right] + \frac{1}{2} \exp \left\{\frac{ux}{D_L}\right\} \operatorname{erfc} \left[\frac{x + ut}{2\sqrt{D_L t}}\right] \qquad (4\text{-}3)$$

This solution was computed in the computer program by SUBROUTINE USEX1. For each time level it is computed and printed out at eleven points, equally spaced on $0 \leq x \leq \ell_x$.

The computation is terminated when the relative concentration C/C_0 at $x = \ell_x$ exceeds some value CQUIT, which is read in as input data. The value CQUIT = 0.90 was used in all runs.

4.1.1 The Effect of $\alpha_L = D_L/u$

Comparing Runs L-1 and L-3 it is seen that reducing the dispersion coefficient by a factor of 10, keeping all other conditions

RUN	CYCLES	$\frac{\ell_x}{\Delta x}$	ℓ_x (cm)	u (cm/sec)	D_L (cm /sec)	u t/ x			ε_{CN}	Computer Time (sec)
						min	max	step		
L-1	1	100	10.0	0.1	0.01	0.005	5.0	x2.0	0.5	23.8
L-2	-"-	25	-"-	-"-	-"-	-"-	-"-	-"-	-"-	4.0
L-3	-"-	100	-"-	-"-	0.001	-"-	-"-	-"-	-"-	25.2
L-4	3	-"-	-"-	-"-	-"-	-"-	-"-	-"-	-"-	35.3
L-5	1	25	-"-	-"-	0.01	-"-	10	-"-	-"-	3.4
L-6	-"-	-"-	-"-	-"-	-"-	-"-	3.5	x1.5	-"-	10.2
L-7	-"-	-"-	-"-	-"-	-"-	0.5	5.0	x2.0	-"-	2.6
L-8	-"-	-"-	-"-	-"-	-"-	0.005	-"-	-"-	1.0	4.2
L-9	3	-"-	-"-	-"-	-"-	-"-	-"-	-"-	-"-	5.1
L-10	-"-	-"-	-"-	-"-	-"-	-"-	-"-	-"-	0.5	5.2
L-11	-"-	100	-"-	-"-	0	-"-	-"-	-"-	-"-	36.0

Table 4-1: Data for Runs for Longitudinal Dispersion in Homogeneous-Isotropic Media

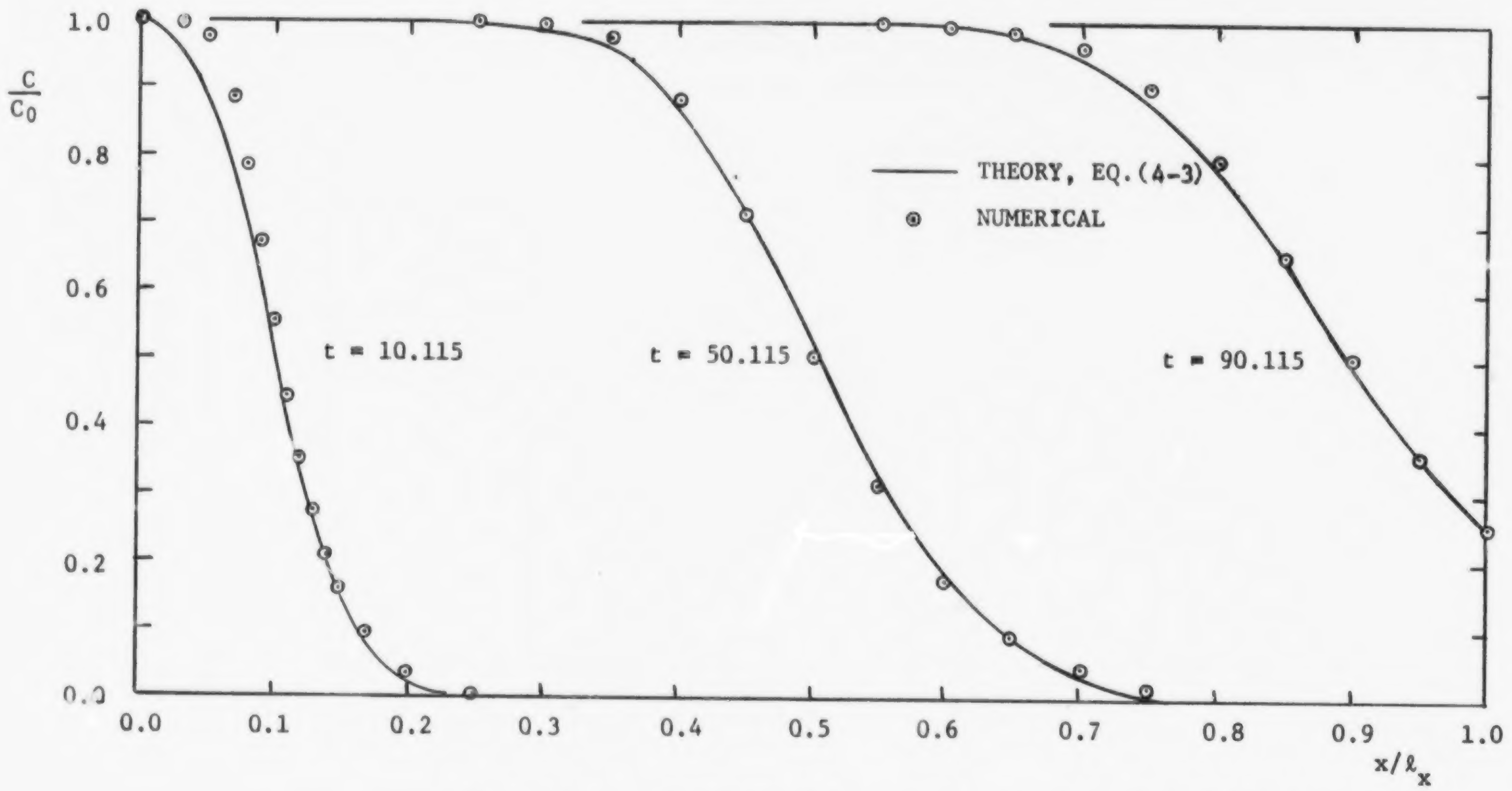


Figure 4-1: Longitudinal Dispersion, Run L-1, (see Table 4-1)

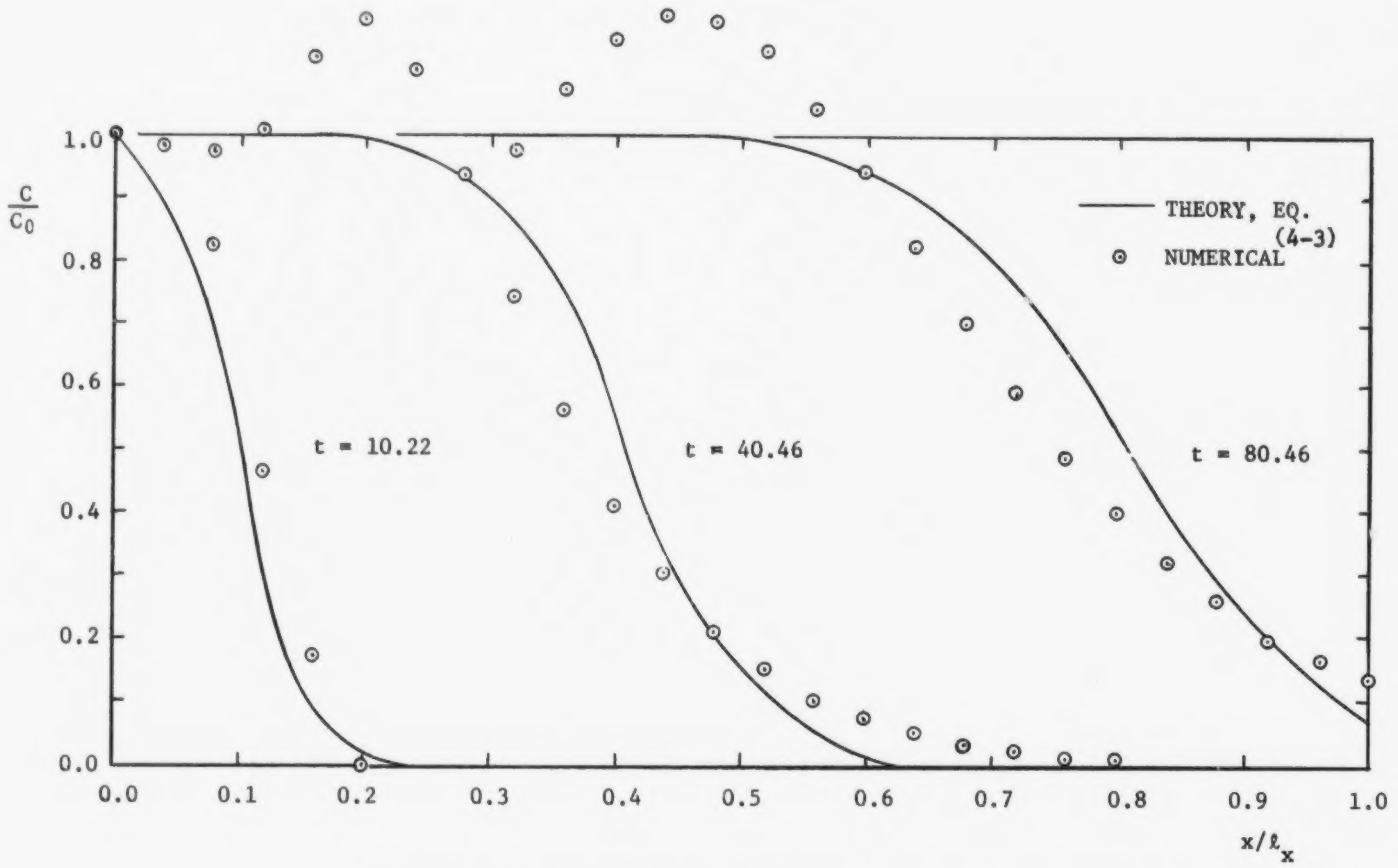


Figure 4-2: Longitudinal Dispersion, Run L-2, (see Table 4-1)

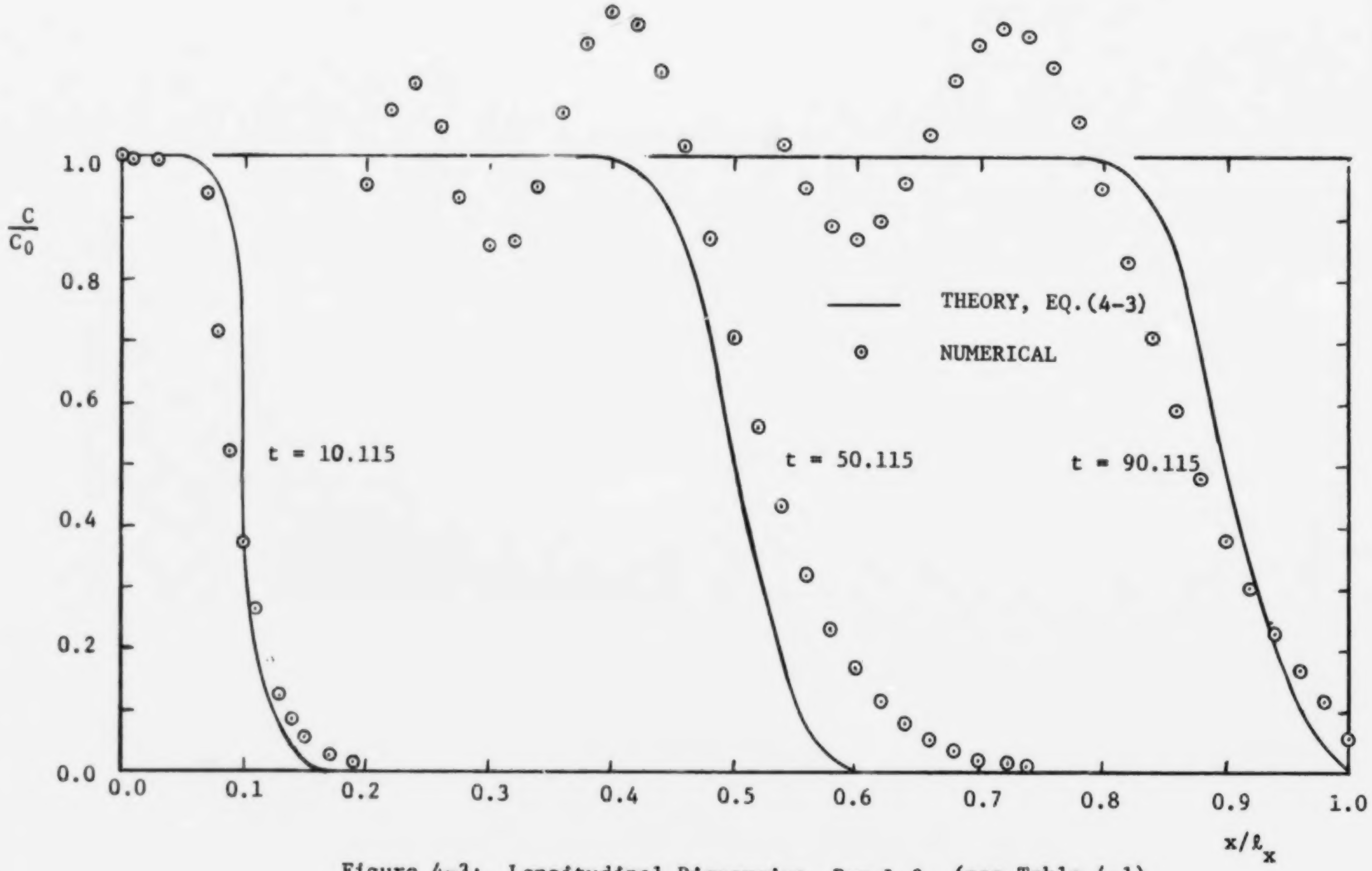


Figure 4-3: Longitudinal Dispersion, Run L-3, (see Table 4-1)

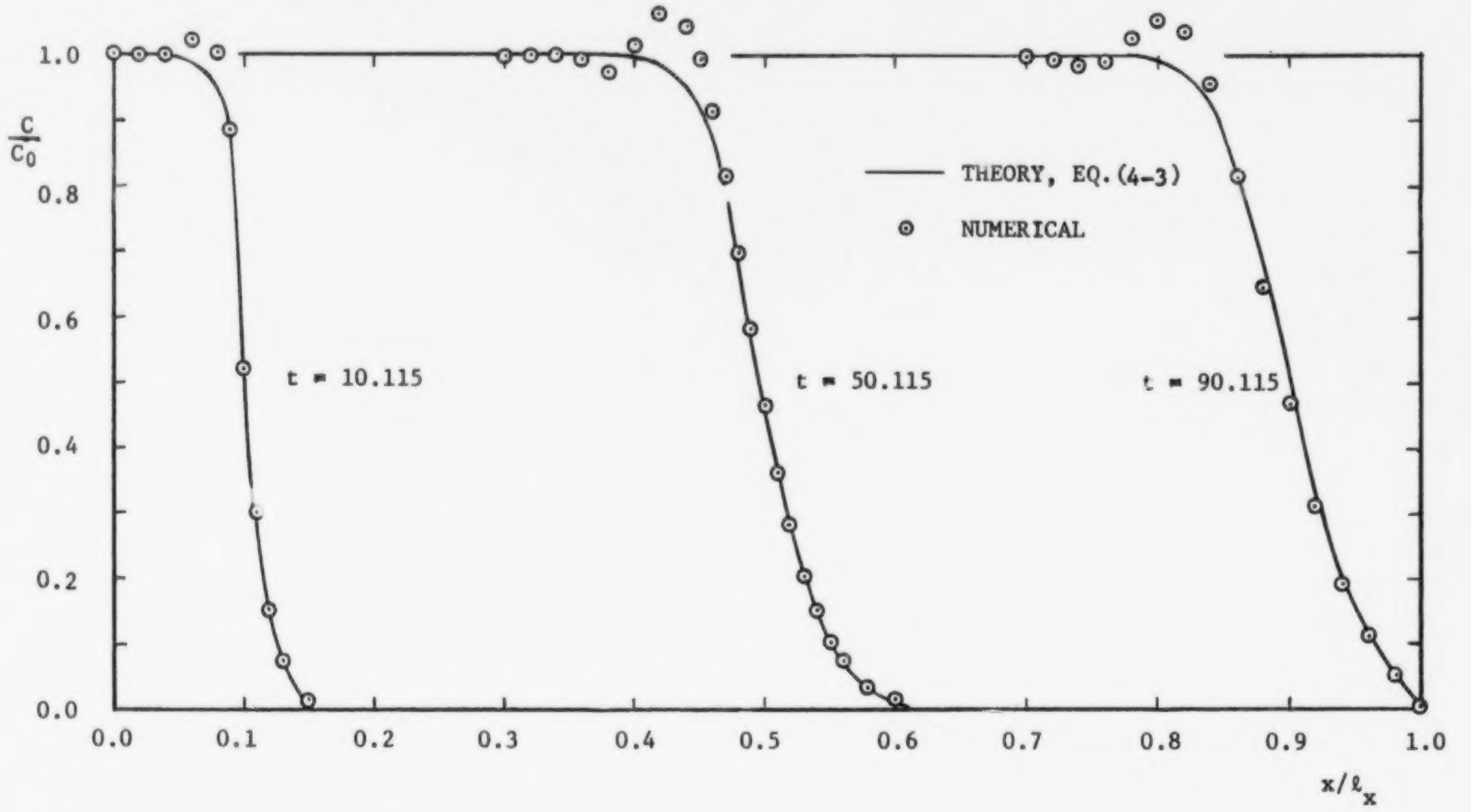


Figure 4-4: Longitudinal Dispersion, Run L-4, (see Table 4-1)

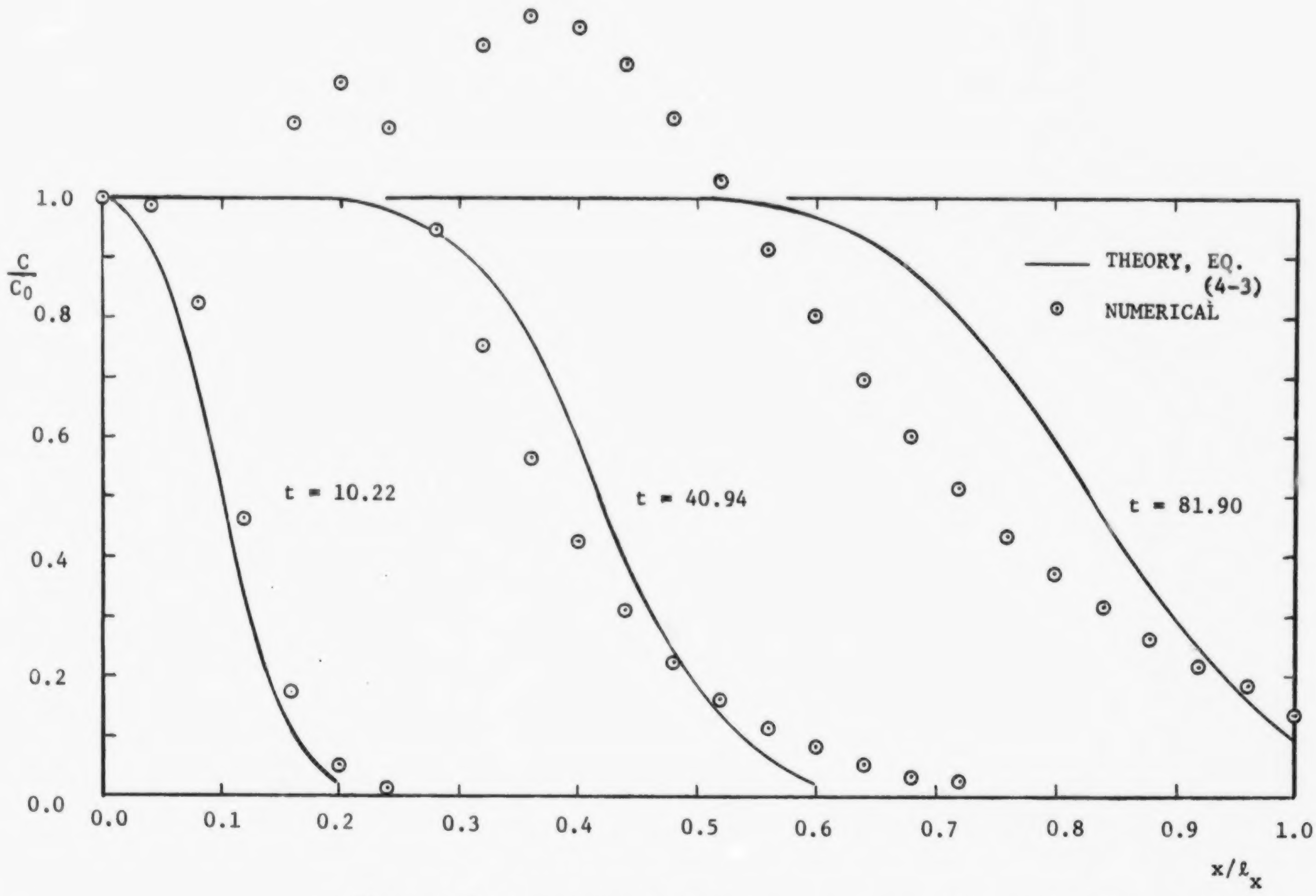


Figure 4-5: Longitudinal Dispersion, Run L-5, (see Table 4-1)

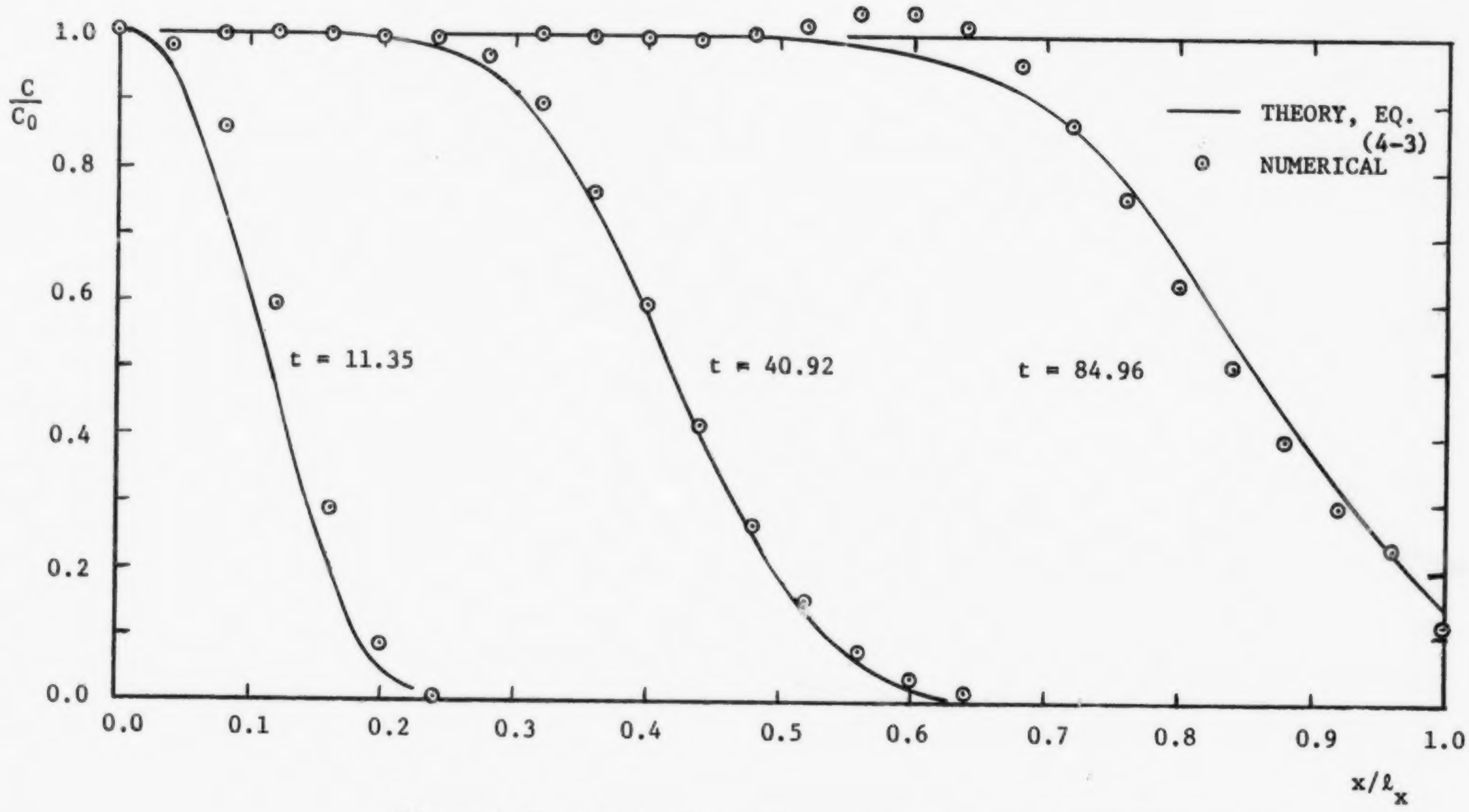


Figure 4-6: Longitudinal Dispersion, Run L-6 , (see Table 4-1)

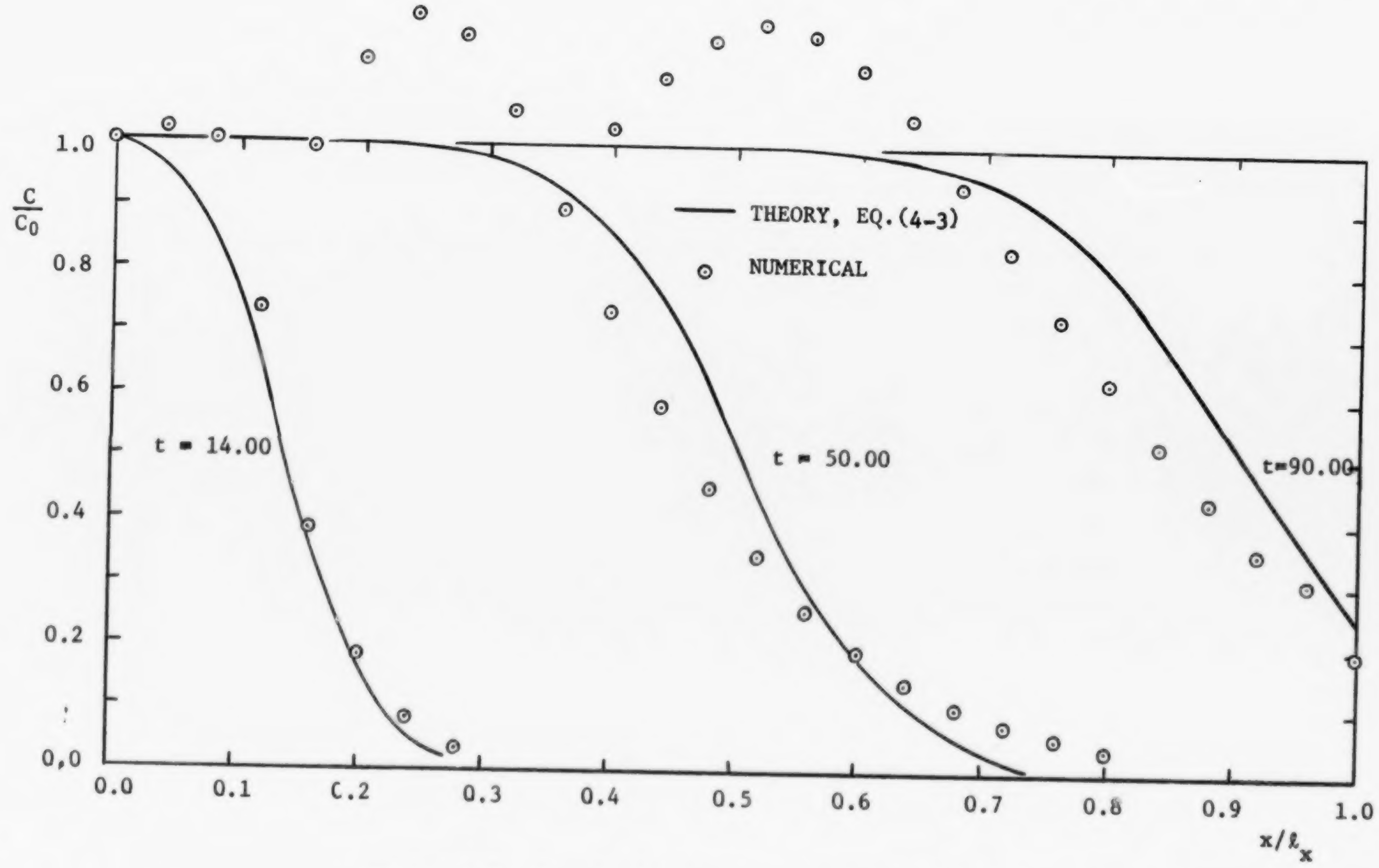


Figure 4-7: Longitudinal Dispersion, Run L-7, (see Table 4-1)

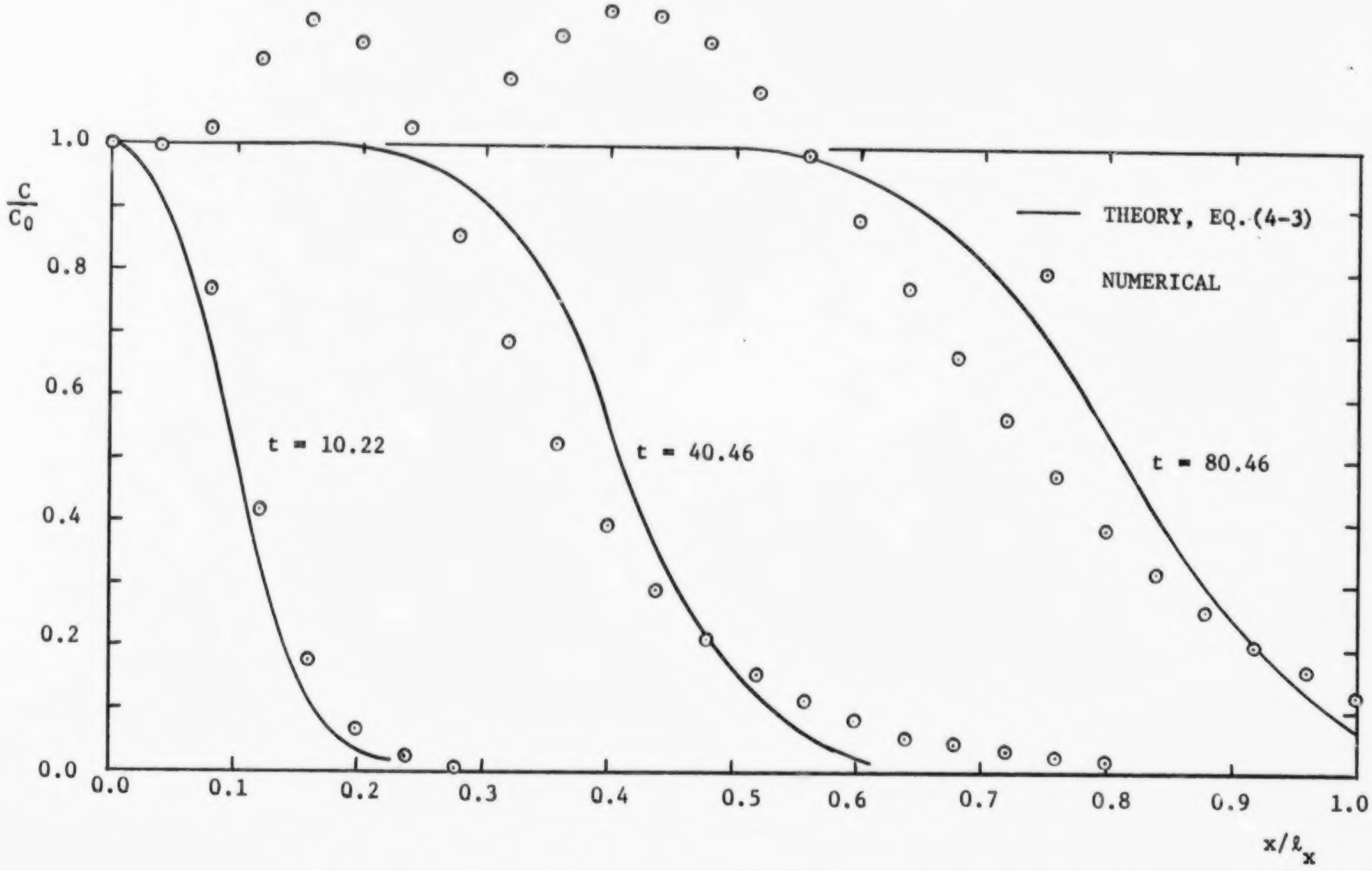


Figure 4-8: Longitudinal Dispersion, Run L-8, (see Table 4-1)

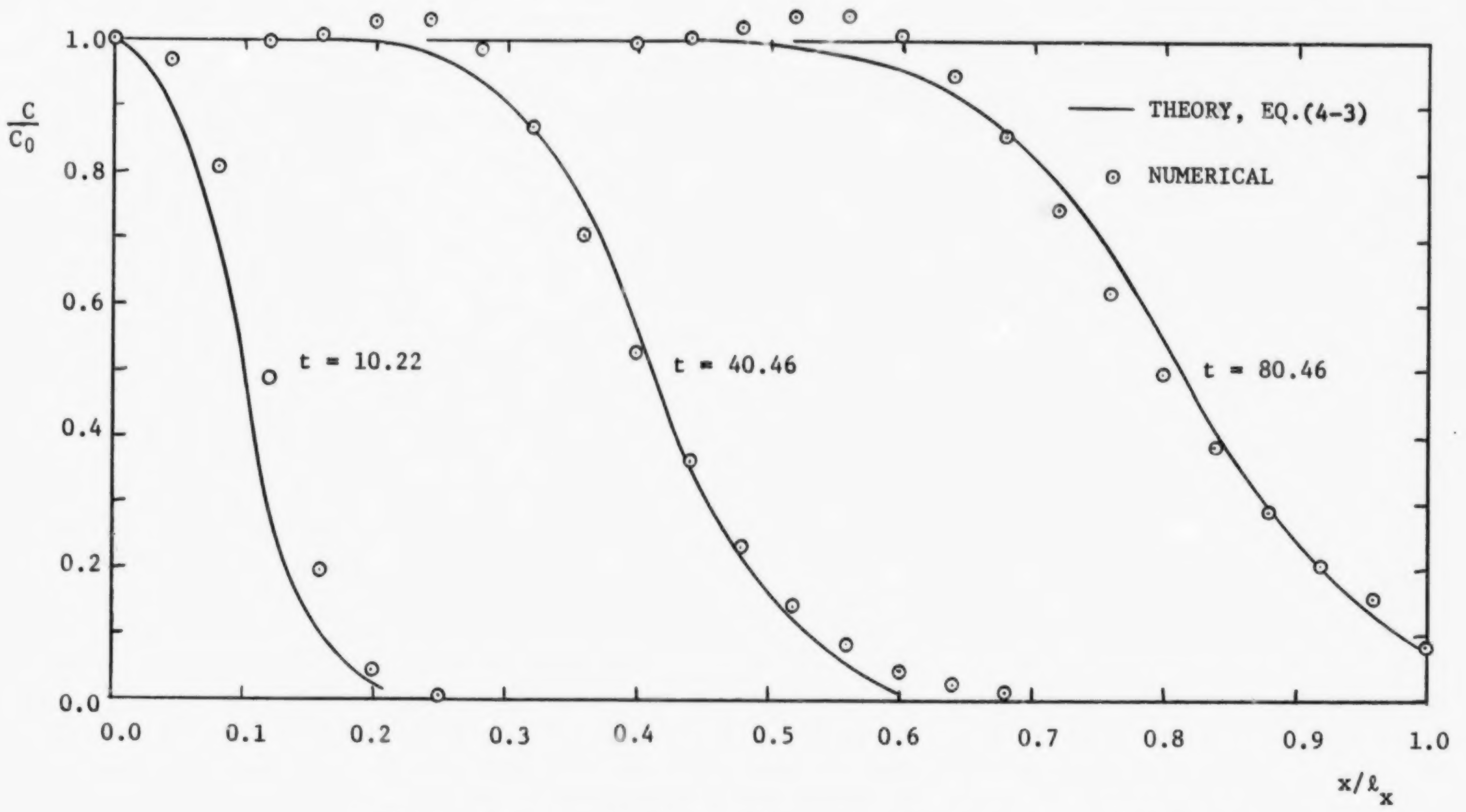


Figure 4-9: Longitudinal Dispersion, Run L-9 , (see Table 4-1)

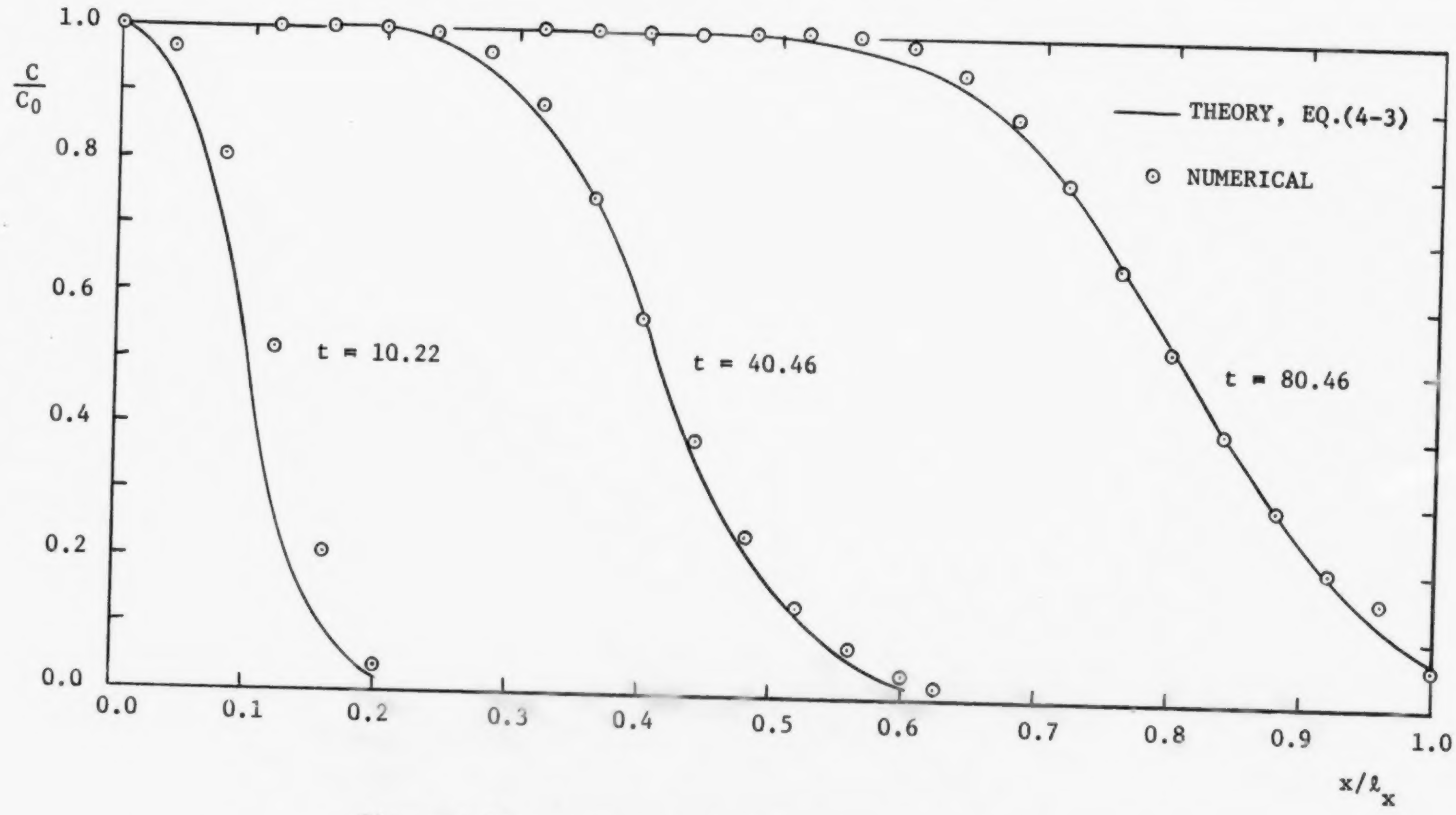


Figure 4-10; Longitudinal Dispersion, Run L-10 , (see Table 4-1)

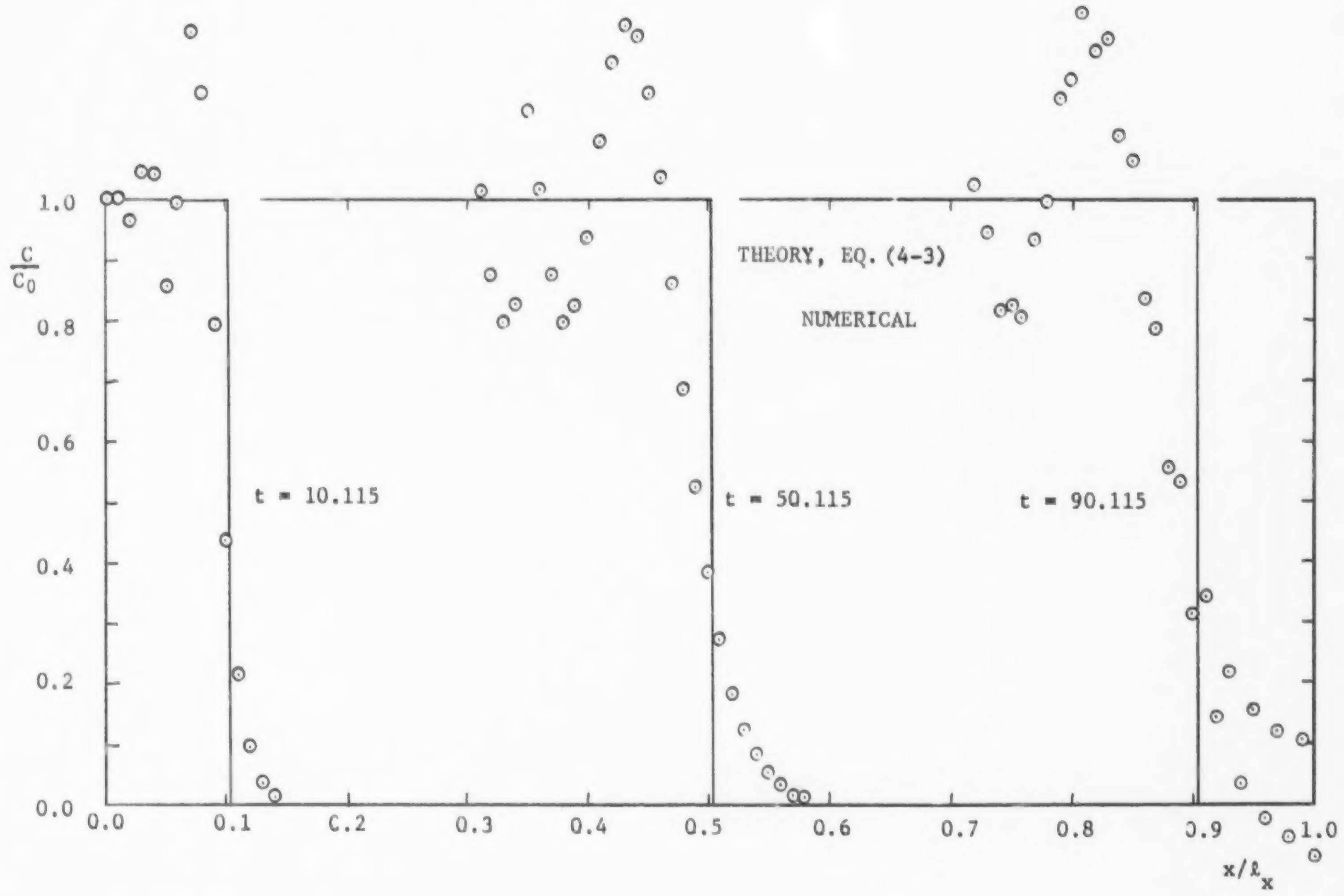


Figure 4-11: Longitudinal Dispersion, Run L-11 , (see Table 4-1)

equal, reduces the accuracy of the solution considerably. The accuracy can be improved for the case $\alpha_L = 0.01$ by using three cycles, as was done in Run L-4. Additional improvement could be achieved by allowing only smaller time steps.

The case $D_L = 0$ causes the greatest difficulty. Even with three cycles the results display large oscillations, as may be seen in Run L-11. The solution is still stable, as the amplitude of the oscillations does not increase with time. The "overshoot" behind the front is about 30% at all times. It is interesting to note that the point $C/C_0 = 0.5$ moves approximately with the flow velocity, u.

4.1.2 Effect of the Number of Cycles

Comparing Runs L-2 and L-10 it is seen that using three cycles instead of one changes the accuracy for certain cases from unacceptable (Run L-2) to satisfactory (Run L-10), at the cost of very little additional computer time. The results for Run L-10 are almost as good as those of Run L-1, while the computer time required is less than one quarter.

The three cycle scheme is especially useful when the value of α_L is small.

4.1.3 Effect of ε_{CN}

ε_{CN} is the weighting coefficient in the difference analogue of the second derivative, equation (3-8). The subscript CN is to denote that this is the generalized Crank-Nicholson expression. From Runs L-9 and L-10 it is seen that $\varepsilon_{CN} = 0.5$ gives slightly better results than $\varepsilon_{CN} = 1.0$.

4.1.4 Effect of the Boundary Condition at $x = \ell_x$

A reflection boundary condition at $x = \ell_x$ was used in all runs. This implies a zero slope in the spatial distribution of concentration at the end of the medium (see Section 3.5). This condition is not strictly correct. If an approximate solution to the one dimensional case, equation (5-5), is used, the spatial gradient of concentration at any x is given by

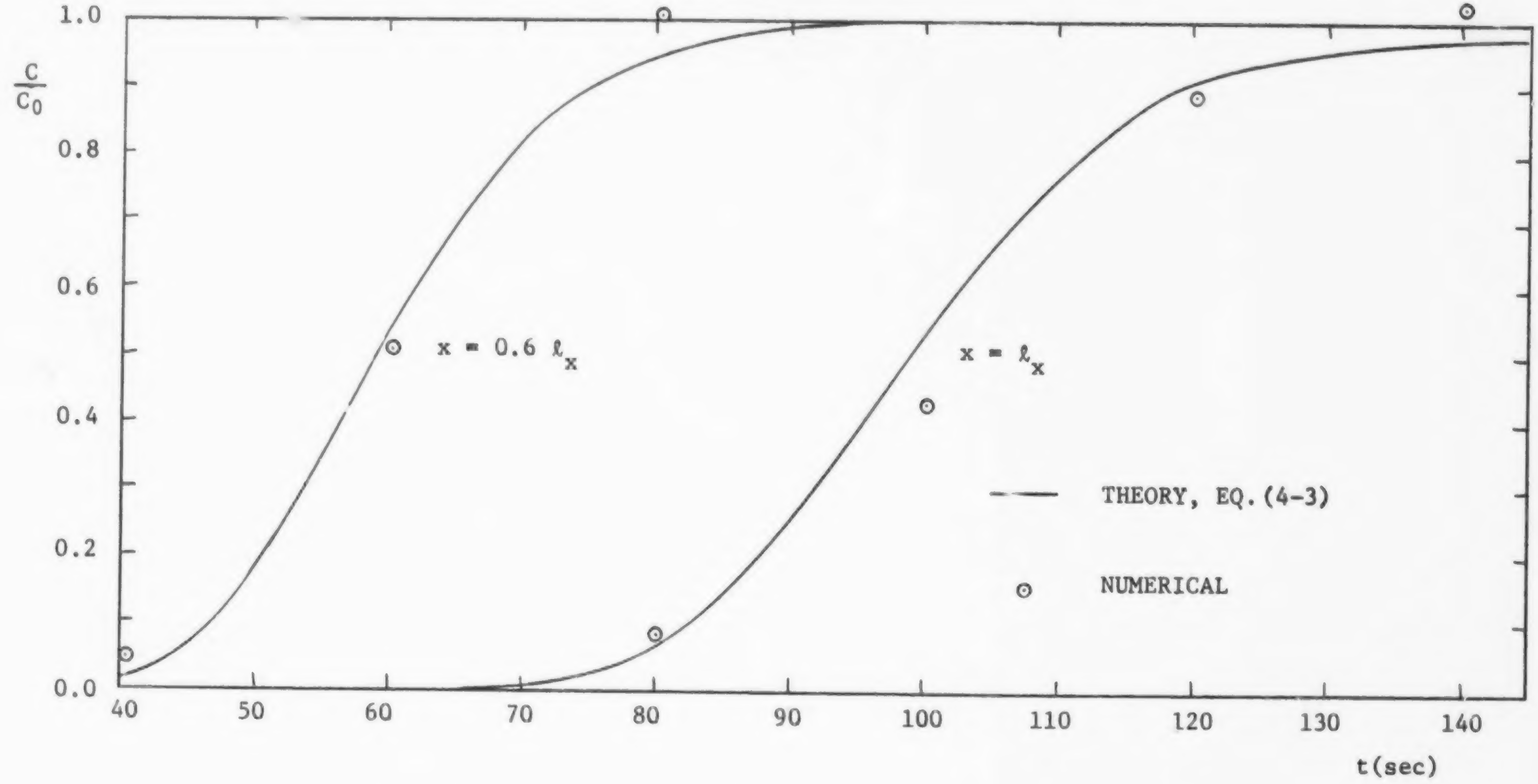


Figure 4-12: Longitudinal Dispersion, Breakthrough Curves at Two Points, Run L-9, (see Table 4-1)

$$\frac{\partial(C/C_0)}{\partial x} = \frac{-1}{\sqrt{\pi D_L t}} \exp\left\{-\frac{(x-ut)^2}{4D_L t}\right\} \tag{4-3}$$

which is never zero for a finite time. It was found that a reflection condition at $x = \ell_x$ gave better results than a transmission condition (which implies a continuation of the slope). However, the results at $x = \ell_x$ are not as accurate as the results for a point inside the media, as can be seen in Figure 4-12. If one is interested especially in the breakthrough curve for $x = \ell_x$ the results can be improved. This can be done by artificially extending the media beyond its physical length. An additional length of the same material is added on, for the purpose of the calculation, and the point $x = \ell_x$ thus becomes an interior point of the new (longer) medium. The breakthrough curve at $X = \ell_x$ is then of the same accuracy as at any other interior point. This procedure was used for longitudinal dispersion in layered media (see Section 5.3.2).

4.1.5 The Time Step Sequence

The efficiency and accuracy of the proposed scheme is strongly dependent on the number of cycles used and the time step sequence.

The experience gained during this investigation is not sufficient to suggest the optimal time step sequence for all cases. It was found, however, that the schemes which were found successful in the one-dimensional case are a good starting point for two-dimensional cases.

The time step sequence for Runs L-1 to L-11 is given in Table 4-1. The initial value $u\Delta t/\Delta x = 0.005$ was found to be satisfactory. Δt was usually multiplied by 2.0 in each step. In Run L-6 the time step was multiplied by 1.1. This improved the results over those of Run L-2, but at a cost of an increase of computation time. Run L-9, which uses three cycles and a multiplier of 2.0, gave the same accuracy as Run L-6, and required only one half of the computation time.

An increase of the initial value for $u\Delta t/\Delta x$ over 0.005 reduces the accuracy somewhat, especially at small times, while the saving in computer time is small. Comparing two cases in which $(u\Delta t/\Delta x)_{max}$ is 5.0 and Δt is increased by a factor of 2.0 at each step, if the initial value of $(u\Delta t/\Delta x)$ is 0.005 it takes 10 steps to reach the maximum value, and 4 steps if the initial value is 0.5. This difference is small, compared with the total number of steps needed in any two-dimensional problem.

4.1.6 A Random Permeability Distribution

It is clear that the concept of a homogeneous porous medium, when applied to bodies of packed sand, is a purely theoretical one. Not only are natural aquifers non-homogeneous, but even laboratory models which are constructed under closely controlled conditions have some non-homogeneity. This is caused by segregation of size fractions during the placing of the media in a test section, or by uneven packing. One may distinguish between two types of non-homogeneities. The one type has a length scale of a few grain diameters, and is random (or pseudo random) in nature. It results from the distribution of grain sizes present in the media. The other type is of a much larger scale. In it one may distinguish whole regions with different properties. This type includes a layered medium, which is discussed in Chapter V.

The only way to take into account the first type of non-homogeneity is to consider it random. From tests in the laboratory or in the field one obtains a single value for the permeability of the porous medium. This value is obtained under the assumption that the medium is homogeneous. Actually it is an average value.

To examine the effect of an assumed random distribution of permeabilities one may superpose on the average value a random fluctuation with some range. The formula for the local permeability is then given by

$$k = \bar{k}\,(1 + \mu r^*) \qquad (4\text{-}4)$$

where k = local permeability

$\bar{k}$ = spatial average permeability

r^* = a random variate uniformly distributed between $-1/2$ and $+1/2$.

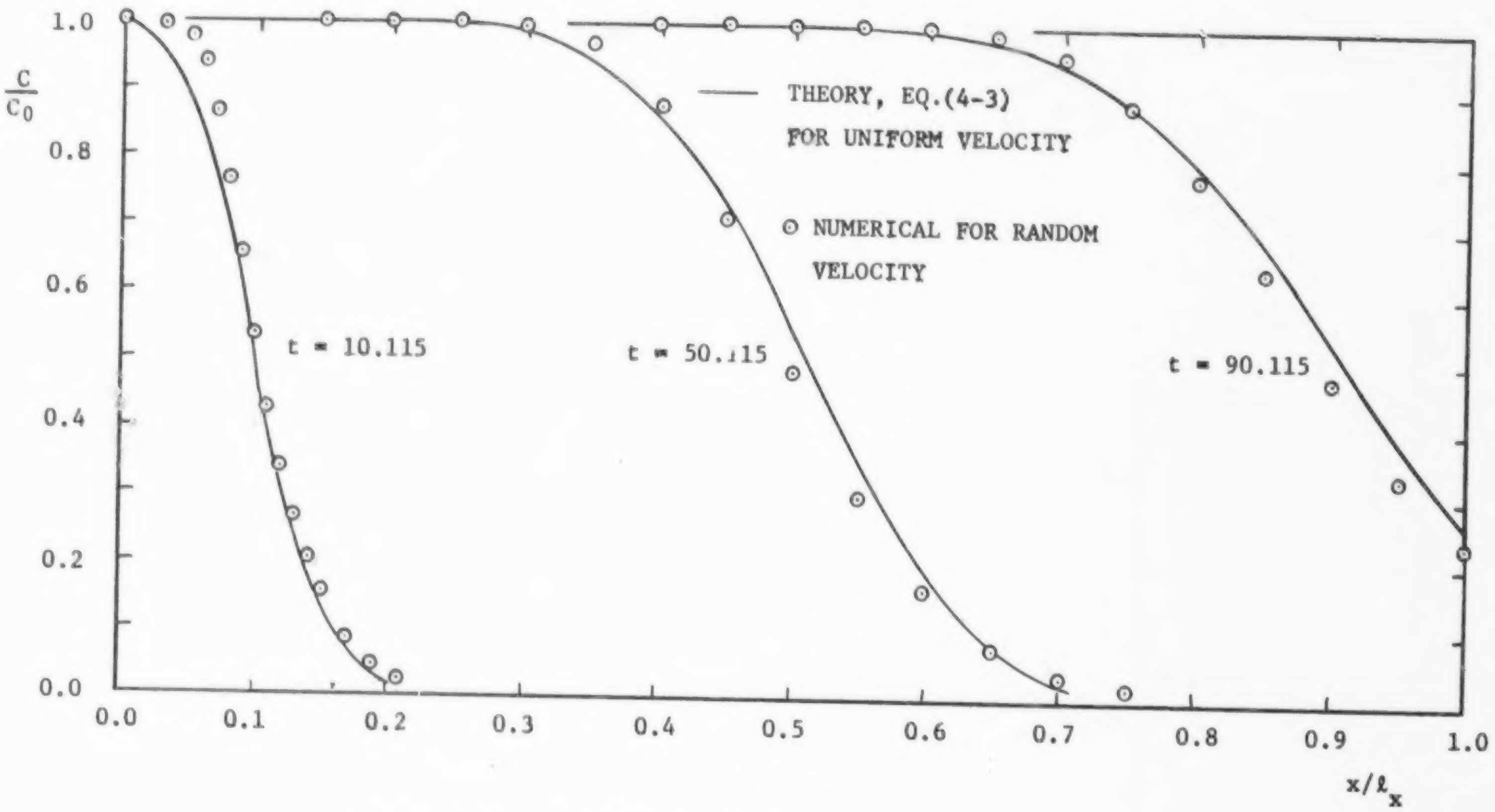


Figure 4-13: The Effect of a Random Distribution of Permeabilities, Run LR-2

μ = the range of variation.

This was incorporated in the one-dimensional program by considering the velocity as given by a similar formula, namely

$$u = \bar{u}\,(1 + \mu r^*) \tag{4-5}$$

and keeping the relation

$$D_L = \alpha_L\, u \tag{4-6}$$

which relates the local dispersion coefficient to the local seepage velocity.

Figure 4-13 shows the results of Run LR-2. All the data are the same as in Run L-1 except that $u = 0.10\,(1 + 0.10r^*)$, and $D_L = 0.10\, u$. The actual mean seepage velocity turned out to be $\bar{u} = 0.9921$.

The random variate was generated by an IBM library subroutine (RANNOF), which uses the power residue method.

The results are very similar to those of Run L-1, although the seepage velocity varies by as much as 5% on either side of the mean.

4.2 Longitudinal Dispersion in Unsteady Uni-Directional Flow

The proposed scheme was developed primarily for problems with steady flow. It may be applied, however, to some cases of unsteady flow as well. Consider the one-dimensional problem discussed in Section 4.1, but with a seepage velocity which is a function of time. At any instant the velocity is the same at every point in the field. Consider the n th time level of the numerical solution. The initial condition for this time interval is the spatial distribution of concentration which resulted from the solution of the (n-1)st time level. The scheme can handle any type of initial condition, so if some new seepage velocity is assigned at the n th time level the solution can be propagated as if the flow were steady during this interval of time. The only restriction that should be imposed on the numerical solution is that the time step used be

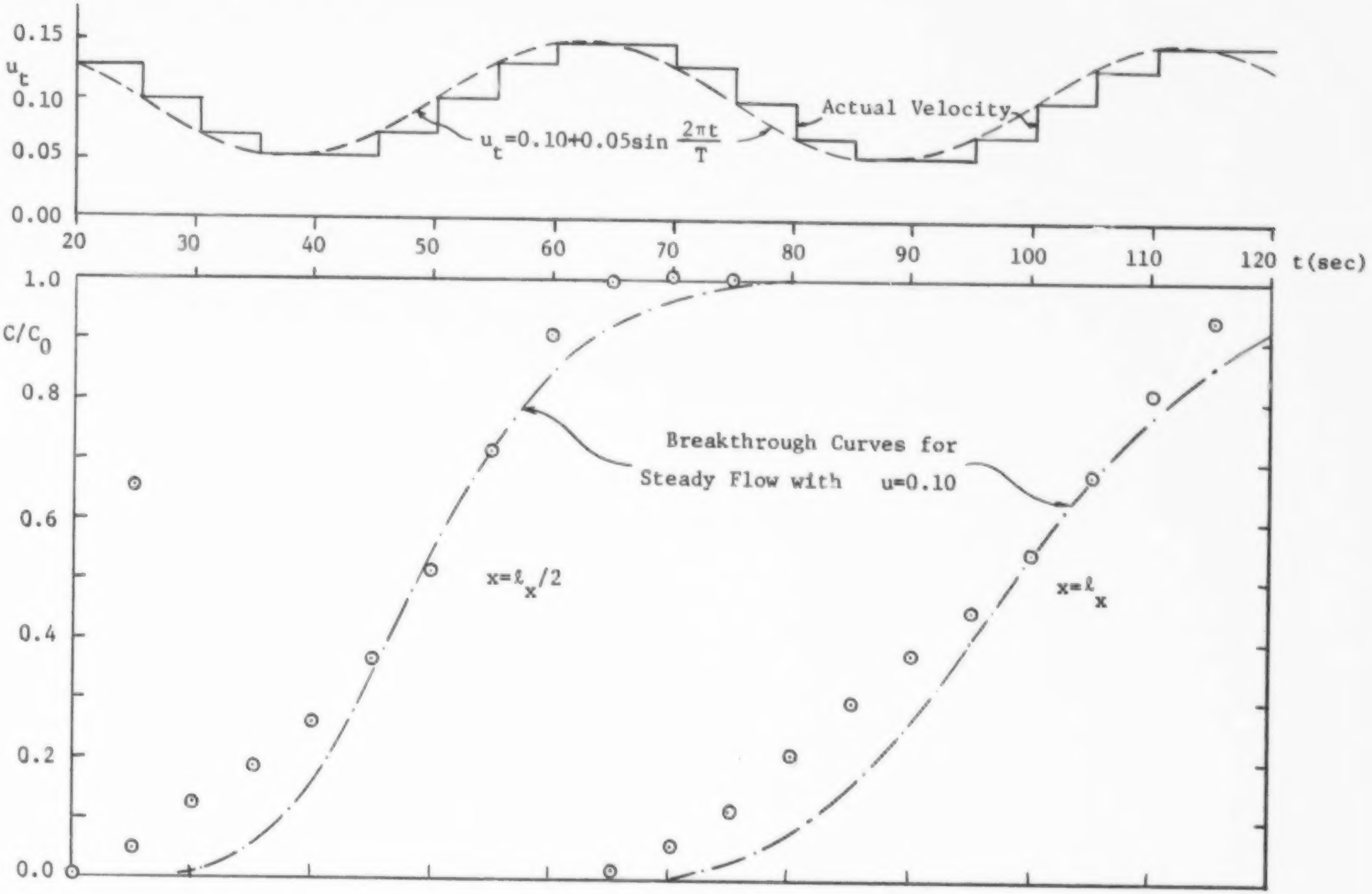


Figure 4-14: Longitudinal Dispersion in Unsteady Flow, Run LUF-1

small compared with the time scale of variation of the seepage velocity. This merely assures that the velocities used in the solution follow closely the actual velocity variation (see Figure 4-14).

The proposed scheme can be applied with no modification to cases with unsteady flow only when the streamlines and equipotentials do not shift position with time. This is clearly the case for the one-dimensional unsteady flow described above, if the total potential is always divided into the same number of drops. The location of each equipotential is fixed, although the numerical value of Φ associated with each equipotential varies with time. The same is true for the streamlines.

This condition is also satisfied in the cases of radial flow and source-sink flow in a confined aquifer with no natural flow. Further discussion of unsteady flow in these cases is included in Sections 4.3 and 4.5.

To demonstrate the use of the scheme for unsteady flow the case of uni-directional flow with sinusoidally varying seepage velocity was used. The instantaneous velocity is given by

$$u_t = u + u_a \sin \frac{2\pi t}{T} \tag{4-7}$$

where u = the time average velocity

u_a = the amplitude of the variation in the velocity

T = the period of the oscillation in the velocity.

The longitudinal dispersion coefficient is assumed to be given by

$$D_{L_t} = \alpha_L u_t \tag{4-8}$$

There is no experimental evidence on the validity of relation (4-8) for unsteady flows. If the velocity does not change rapidly, it is reasonable to use for unsteady flow the same relation as for steady flow.

Figure 4-14 gives the results of Run LUF-1, for which the velocity is

$$u_t = 0.10 + 0.05 \sin \frac{2\pi t}{50}$$

and $$\alpha_L = 0.10$$

All other data are the same as for Run L-1. The breakthrough curves for steady flow with u = 0.10 and α_L = 0.10 are given in the figure as a reference. The actual velocity variation used in the solution is also shown in Figure 4-14.

4.3 Radial Flow

The advantages of using the convective dispersion equation in Φ-ψ coordinates were outlined in Chapter III. One of these was the statement that the weighting scheme developed by Stone and Brian for the one-dimensional case is applicable, without modification, to the convective and time terms of the two-dimensional equation written in Φ-ψ coordinates. The present section serves as a demonstration of this point.

Consider a well, fully penetrating a confined aquifer of thickness b, made of a homogeneous-isotropic medium. The well recharges into the aquifer a steady discharge Q, and the flow in the aquifer is due only to the well discharge. The flow is axisymmetric, and if the input concentration is axisymmetric as well (e.g. a step change of concentration in the well) then equation (2-11) is the convective dispersion equation for this case. Equation (2-11) is one dimensional in cylindrical coordinates, but it is non-linear.

One may try to solve equation (2-11) numerically. The r-axis is then divided into equal increments Δr. The velocity at each point is $q_r = A/r$. Thus, when a point at radius r_1 is considered, the velocities at the points on either side of it are $A/(r_1 - \Delta r)$ and $A/(r_1 + \Delta r)$. The product $q_r \Delta r$ is not equal for these two points, so they have unequal "weight" relative to point under consideration. If, on the other hand, the radial flow problem is solved numerically by using the Φ-ψ equation, the Φ-axis (which is directed radially outward) is divided into equal increments $\Delta\Phi$. Then

$$\Delta\Phi = \text{const} = \Delta(A \ \ell nr) = A \ \Delta(\ell nr) \qquad (4\text{-}9)$$

leads to

$$\Delta r = r(e^{\Delta\Phi/A} - 1) = K_1 r \qquad (4\text{-}10)$$

and

$$q_r \Delta r = \frac{A}{r} K_1 r = K_2 \qquad (4\text{-}11)$$

where K_1 and K_2 are constants.

The Stone and Brian scheme was used to compute a numerical solution of both equations, in radial coordinates and in Φ-ψ coordinates. The weighting coefficients for both equations were the same as in the one-dimensional case with one cycle, namely

$$a_1 = a_2 = a_3 = a_4 = 0.25$$

and $$b_1 = 0.6667, \quad b_2 = b_3 = 0.1667$$

The same time step sequence was used in both cases. The results are compared in Figure 4-15, in the non-dimensional coordinate $\rho = r/\alpha_L$ and the non-dimensional time $\tau = At/\alpha_L^2$. The heavy lines are the approximate analytical solution given by Hoopes and Harleman [32]

$$\frac{C}{C_0} = \frac{1}{2} \operatorname{erfc} \left[\frac{\rho^2/2 - \tau}{\sqrt{\frac{4}{3} \rho^3}} \right] \qquad (4\text{-}12)$$

The numerical solution of the Φ-ψ equation agrees very well with the approximate analytical solution, equation (4-12). The numerical solution of the equation in radial coordinates displays large oscillations, and deviates largely from the solution given by equation (4-12). These results support the statement that if one uses the Φ-ψ equation, Stone and Brian's scheme is applicable without modification.

The difference between the numerical results obtained from the two equations is accentuated in the problem presented above because the concentration step occurs in a region in which the Φ-ψ equation has more grid points than the equation in radial

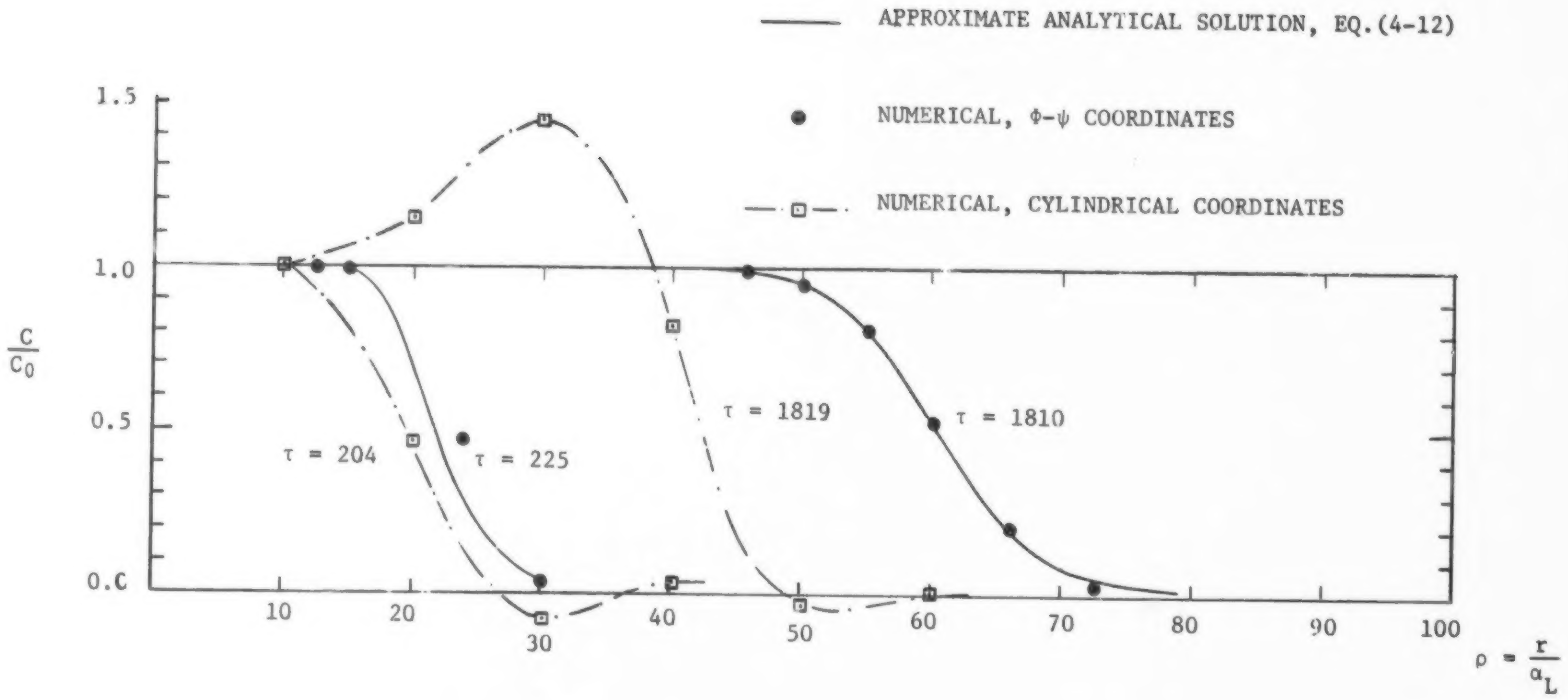


Figure 4-15: Comparison of Numerical Results From Equations in Radial and Φ-ψ Coordinates

coordinates. This increases the accuracy of the former equation. If one were interested in a problem of radially convergent flow to a pumping well, where the step input in concentration is introduced at some sufficiently large radius, then the equation in radial coordinates would have more grid points in the region of large concentration gradients.

It is hard to conceive of a condition in nature in which a step input occurs simultaneously on all streamlines of a converging flow. Usually it will occur at a source of a diverging flow. For this reason the unequal spacing of grid points introduced by the Φ-ψ equation is considered an advantage.

The radial flow problem was solved numerically by Hoopes and Harleman [32]. An explicit scheme was used to solve the equation

$$\frac{\partial C}{\partial \tau} + \frac{1}{\rho}\frac{\partial C}{\partial \rho} = \frac{1}{\rho}\frac{\partial^2 C}{\partial \rho^2} \tag{4-13}$$

which is equation (2-11) in non-dimensional cylindrical coordinates. The increments $\Delta\tau$ and $\Delta\rho$ are restricted by a stability criterion. Two calculations were carried out

a. $\tau = 0$ to $\tau = 1810$ with $\Delta\tau = 1/4$ and $\Delta\rho = 1$. This computation took about 30 minutes of IBM 7094 computer time.

b. $\tau = 0$ to $\tau = 8028$ with $\Delta\tau = 4$ and $\Delta\rho = 2$. This computation took about 8 minutes. The results of this computation gave results in the region $\tau < 1810$ which did not agree with equation (4-12) as well as the results of computation (a).

The proposed scheme, using the Φ-ψ equation, required about 20 seconds to reach $\tau = 1810$, 32 seconds to reach $\tau = 8028$, and 4.5 minutes to reach $\tau = 112700$. Results are given in Figures 4-16 and 4-17. The time step sequence was started with $\Delta\tau/\Delta\eta = 0.05$, and was carried to $\Delta\tau/\Delta\eta = 5000$ with $\Delta\tau$ multiplied by 1.3 at successive time steps. The results were absolutely stable (i.e. there was no "overshoot" behind the advancing front), and therefore $\Delta\tau/\Delta\eta = 5000$ is not the maximum possible value. The agreement of these calculations with equation (4-12) is better than

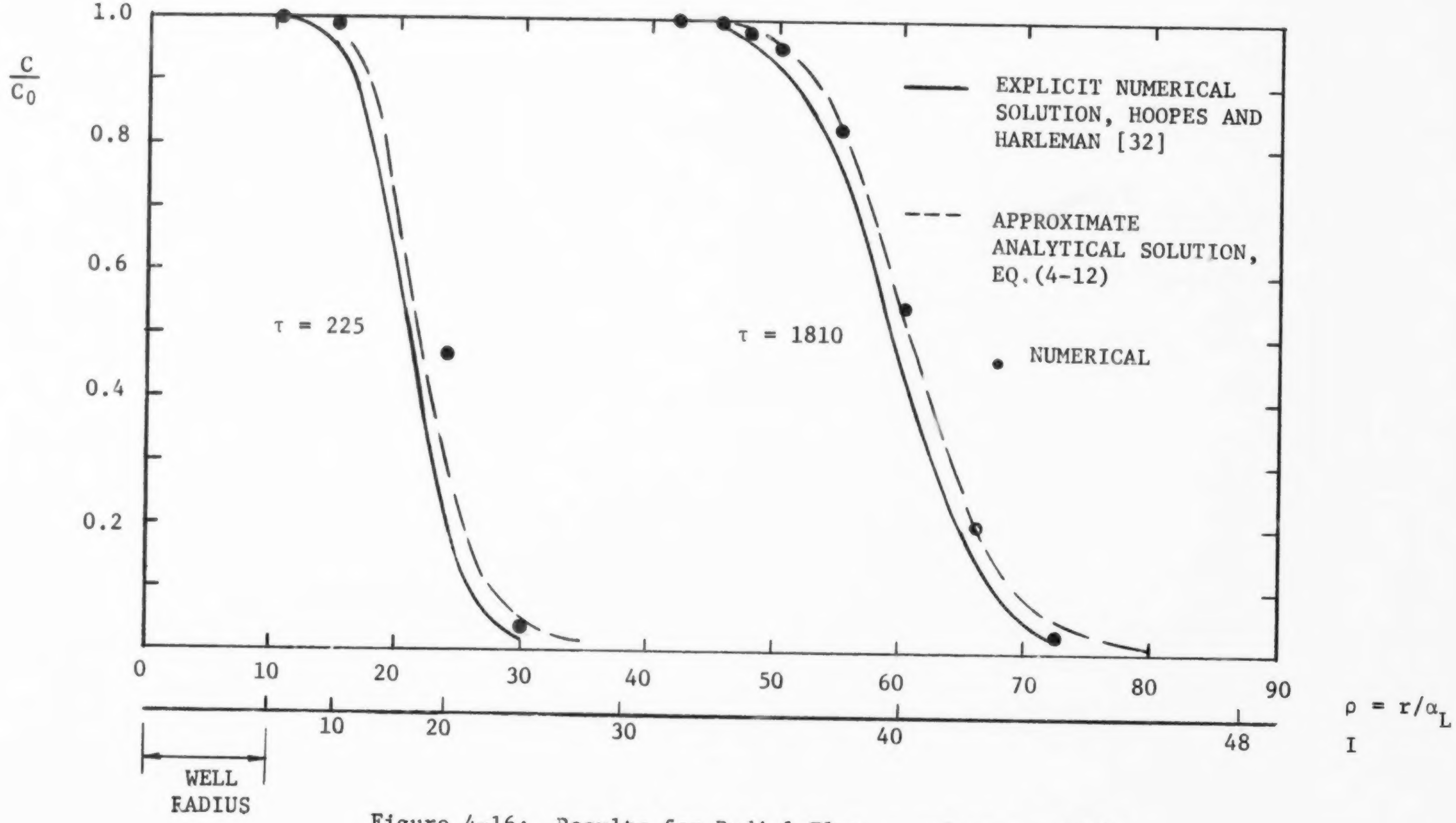


Figure 4-16: Results for Radial Flow, $\tau = 0$ to $\tau = 1810$

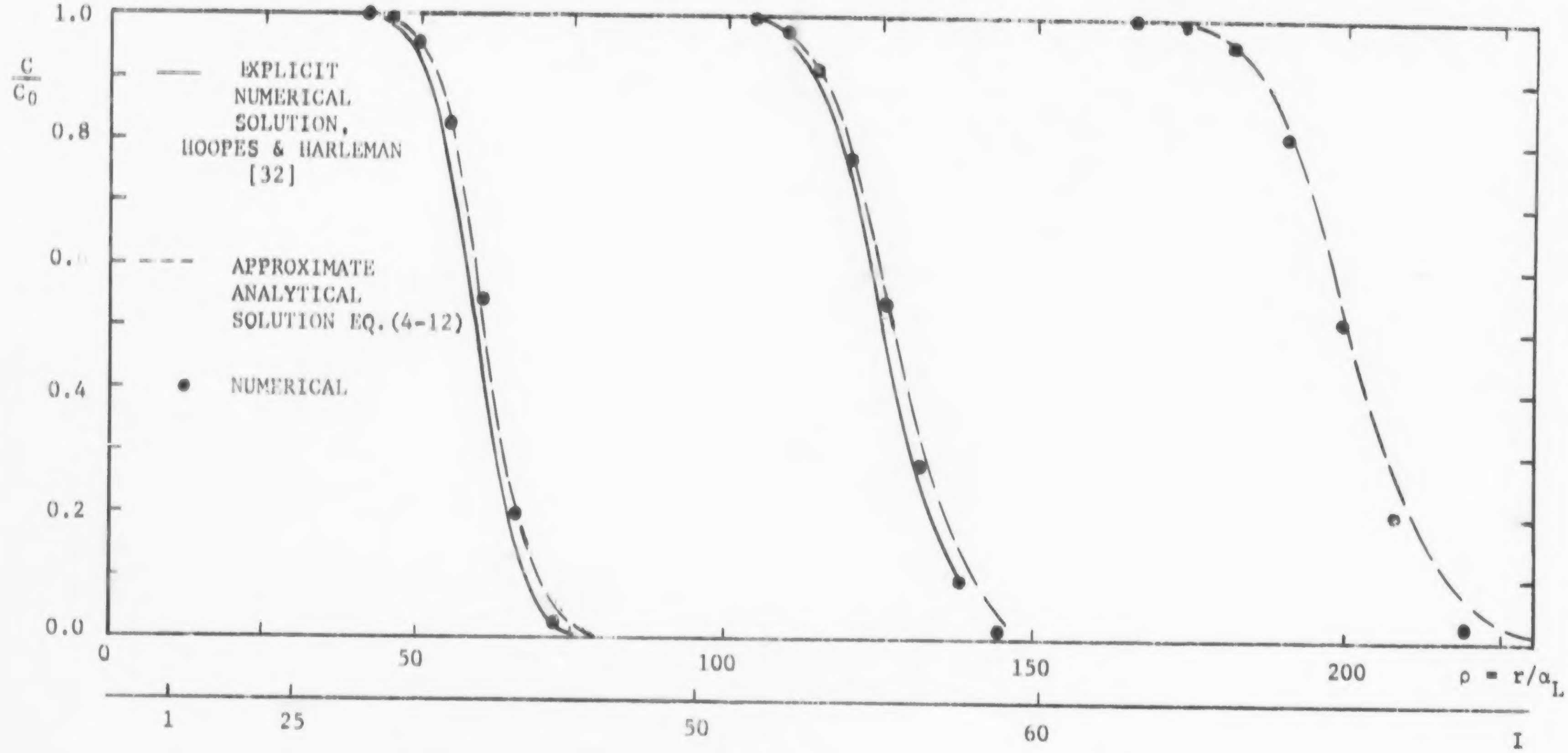


Figure 4-17: Results for Radial Flow, $\tau = 0$ to $\tau = 20070$

that achieved by the explicit solution, except for very small values of τ. It should be noted that even at $\tau = 112700$ the point $C/C_0 = 0.50$ is only at $\rho \cong 480$.

For a well discharging 1 cfs into an aquifer with $b = 100$ ft and $\theta = 0.35$, $A = 4.55 \times 10^{-3}$ ft^2/sec. Then, if $\alpha_L = 0.15$ cm = $= 4.93 \times 10^{-3}$ ft, one gets $t = 5.5 \times 10^{-3}\tau$, and $\tau = 112700$ corresponds to $t \cong 250$ seconds. To carry the solution out to larger values of τ requires larger amounts of computer time.

At this point it should be emphasized that one of the uses of the numerical scheme will be in helping to find approximate analytical solutions to specific problems. If an approximate analytical solution, which is of acceptable accuracy for practical problems can be found, it has advantages over the numerical scheme. First, its calculation is always shorter. Second, the concentration at any point or time can be calculated directly - without having to carry the solution all the way from the initial condition to the desired point. This is the case for the radial flow problem. The numerical scheme has substantiated the approximate analytical solution, and the latter should be used.

The problem of dispersion in unsteady radial flow in a confined aquifer may be solved by the proposed scheme as well. If elasticity of the aquifer is neglected, the lines of $\eta = \phi/A$ = constant maintain their location even when A changes. If the time increments for the numerical solution are taken much smaller than the scale of variation of the velocity, the numerical solution can reproduce the true solution. The velocity varies from one time step to the next, but is considered constant during each time increment.

To demonstrate the ability of the scheme to handle other types of boundary conditions the radial flow problem was solved for a finite pulse input in concentration. The boundary condition at the well is

$$C_{well} = C_0 \qquad 0 \le \tau \le \tau_c$$

$$C_{well} = 0 \qquad \tau_c < \tau$$

where t_c is a finite length of time.

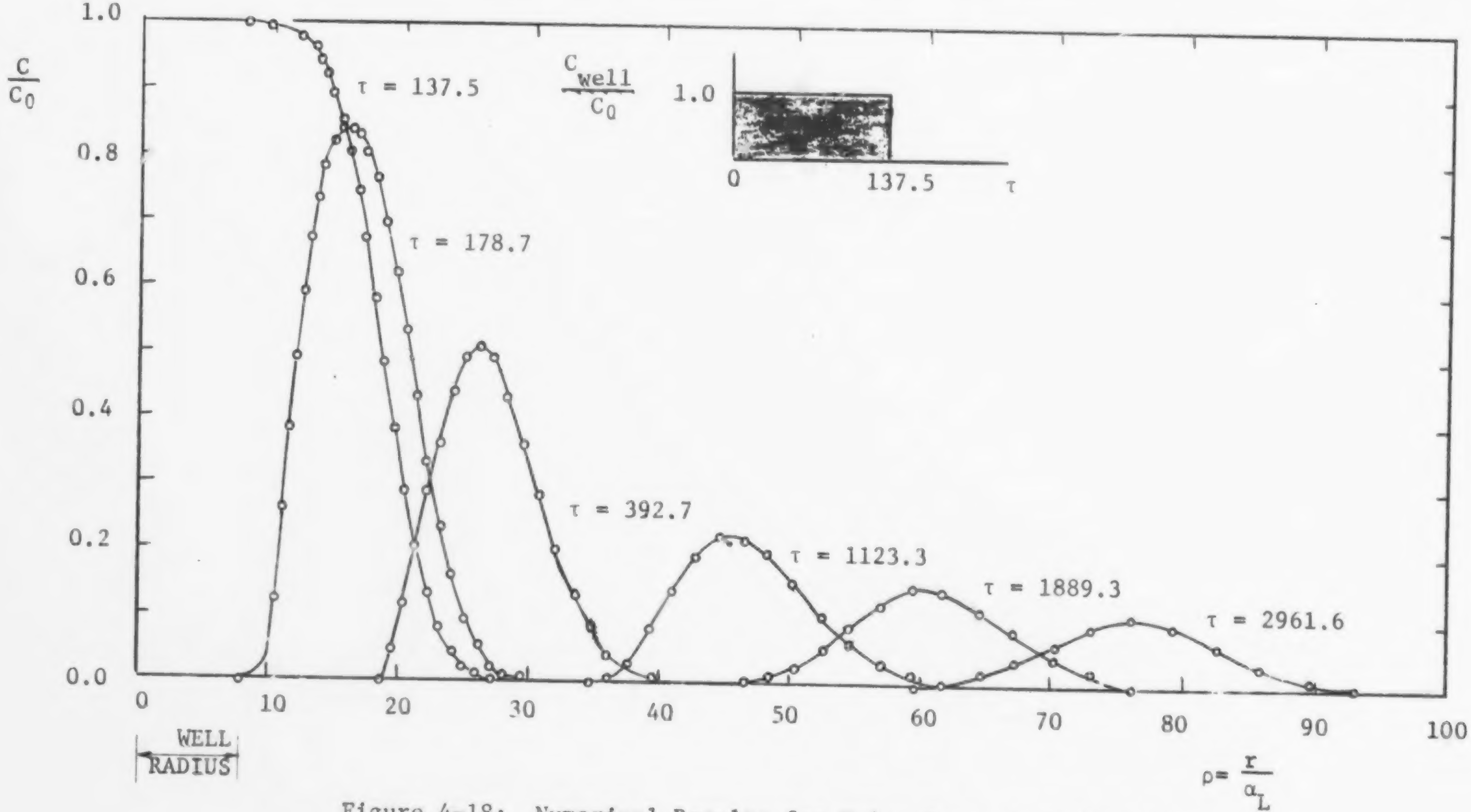


Figure 4-18: Numerical Results for Pulse Input in Radial Flow

There exists no exact or approximate analytical solution to this problem. Results obtained from the numerical scheme for the case $\tau_c = 137.5$ are presented in Figure 4-18, which shows the spatial concentration distribution at some values of τ.

4.4 Longitudinal and Lateral Dispersion in Uni-Directional Flow

Consider the rectangular region $0 \le x \le \ell_x$, $0 \le y \le \ell_y$ in which there is flow along the x-direction with seepage velocity u = constant. Equation (2-8) is the convective dispersion equation for this case. The problem considered in this section is the concentration distribution resulting from the boundary conditions

$$C(0,y,t) = 0 \qquad 0 \le y \le b, \quad t \ge 0$$

$$C(0,y,t) = C_0 \qquad b < y \le \ell_y, \quad t \ge 0$$

and the initial condition

$$C(x,y,0) = 0 \qquad x > 0, \quad \text{all } y$$

see Figure 4-19.

No analytical solution has been obtained for the transient stage in which the front moves through the media and disperses both longitudinally and laterally. If the input concentration on $x = 0$ is maintained for a sufficiently long time the concentration distribution will reach a steady state. Harleman and Rumer [30] have solved this case, after neglecting the longitudinal dispersion term in the differential equation. This can be done because $\partial^2C/\partial x^2$ is very small, as they have showed. The solution for the steady state is

$$\frac{C}{C_0} = \frac{1}{2} \operatorname{erfc} \left(\frac{y - b}{2\sqrt{D_T x/u}}\right) \tag{4-14}$$

The numerical solution does give the transient solution, but there is no way to check its validity as no analytical or experimental results are available. If, however, the lateral dispersion coefficient is small, and the concentration distribution at $y = 0$ is not affected by lateral dispersion, then

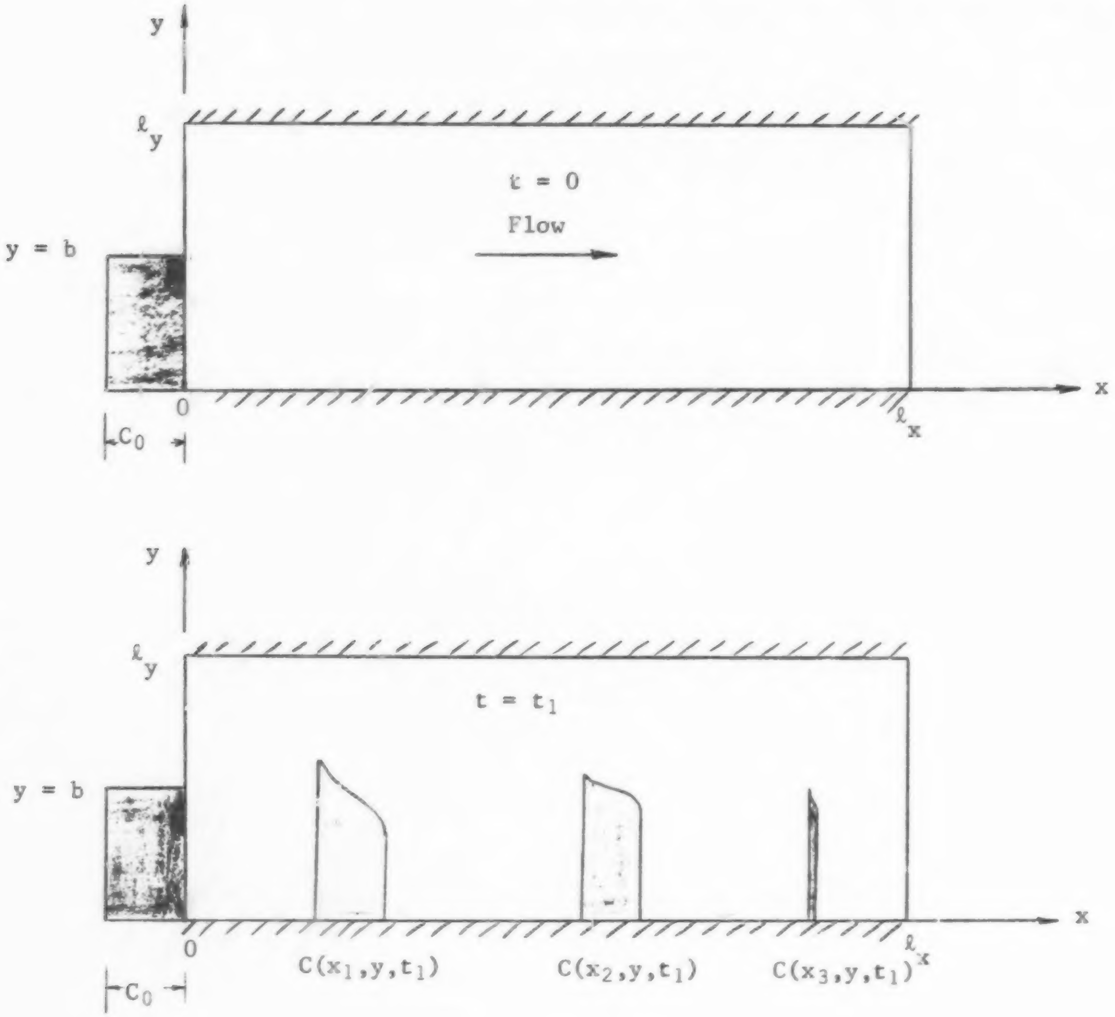

y
ℓ_y
t = 0
Flow
y = b
0
C_0
x
ℓ_x
y
ℓ_y
$t = t_1$
y = b
0
C_0
$C(x_1,y,t_1)$
$C(x_2,y,t_1)$
$C(x_3,y,t_1)$
ℓ_x
x

Figure 4-19: Longitudinal and Lateral Dispersion in Uni-Directional Steady Flow

$$\left.\frac{\partial C}{\partial y}\right|_{y=0} = 0 \tag{4-15}$$

This means that along $y = 0$ the transient concentration distribution is the same as for the one-dimensional case with a step input. One can compare the results along $y = 0$ with the results of the one-dimensional program for the same u, D_L and number of grid points.

The numerical solution was obtained from the full (three equation) scheme with one cycle per time step. Data for Run T-1 are: 25 x 25 slices on $0 \le x \le 10$ cm and $0 \le y \le 10$ cm, $u = 0.1$ cm/sec, $D_L = 0.01$ cm^2/sec, $D_T = 0.001$ cm^2/sec. The time step sequence was given by $u\Delta t/\Delta x = 0.05$ to 5.0 with steps of 1.2. Computer time needed to reach steady state (at about $t = 200$ secs) was 1.5 minutes.

The step in input concentration was located at $y = b = 4.8$ cm. The input concentration for the numerical solution was given by

$$C/C_0 = 1.0 \qquad y < b$$

$$C/C_0 = 0.5 \qquad y = b$$

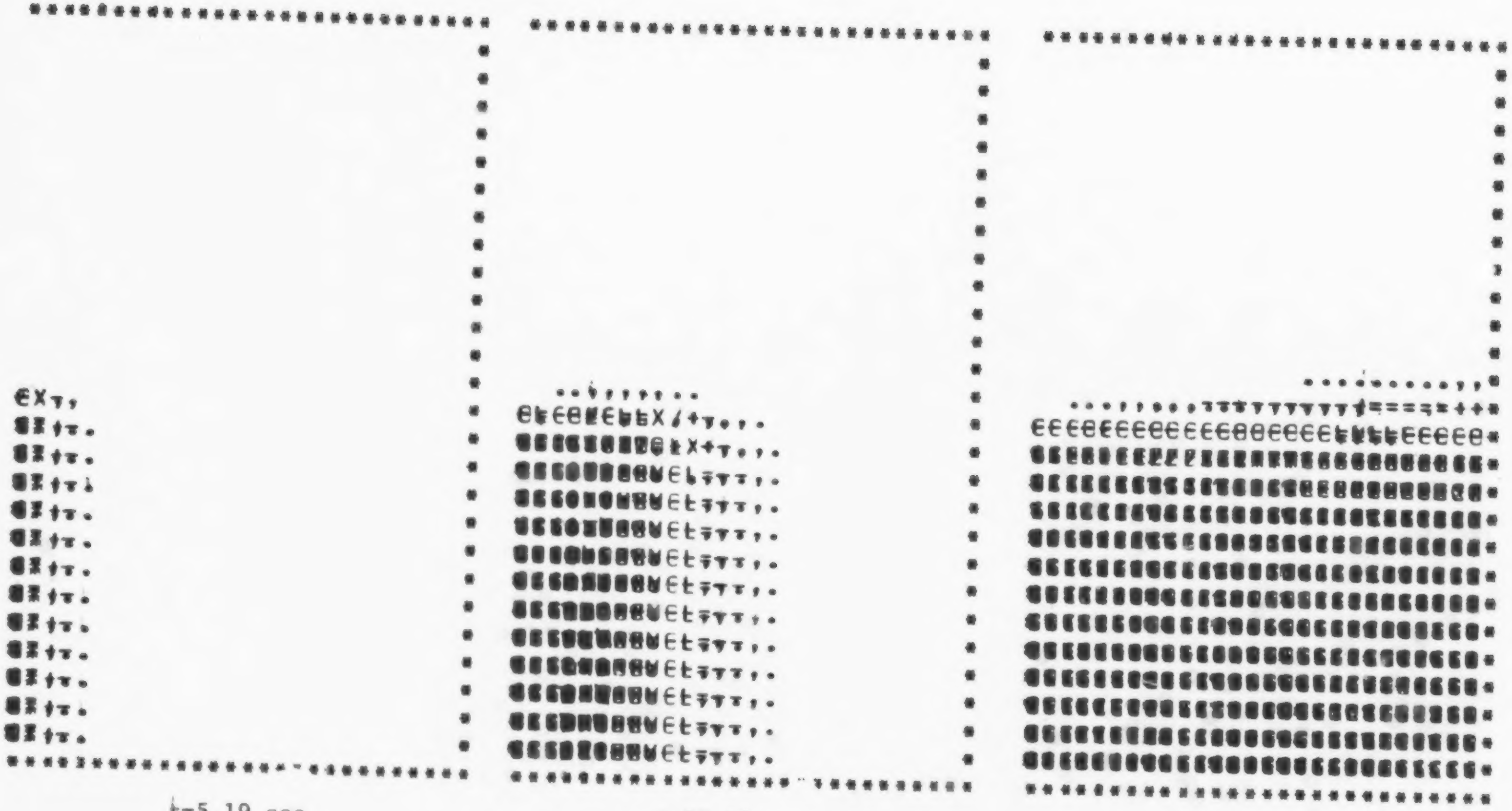
$$C/C_0 = 0 \qquad y > b$$

Using one half the value of the "jump" at the center point is recommended for all cases in which the boundary (or initial) condition has a discontinuity.

The transient results are presented by the output from SUBROUTINE USMAP at three instants of time in Figure 4-20. This output (which is given in addition to the numerical output, and is optional in the program) gives an instantaneous "picture" of the concentration distribution.

The transient concentration distribution at $y = 0$ was identical to the results of the one-dimensional program (1F1D) with the same data. (See note about number of grid points to be used for the comparison in Appendix A.)

The steady state concentration distribution from Run T-1 is compared with the theory, equation (4-14), in Figure 4-21. The accuracy of the numerical results is not satisfactory, and is due to the large spacing of grid points in the y-direction relative



t=5.19 sec

t=37.34 sec

t=182.19 sec

Figure 4-20: Transient Concentration Distribution, Run T-1

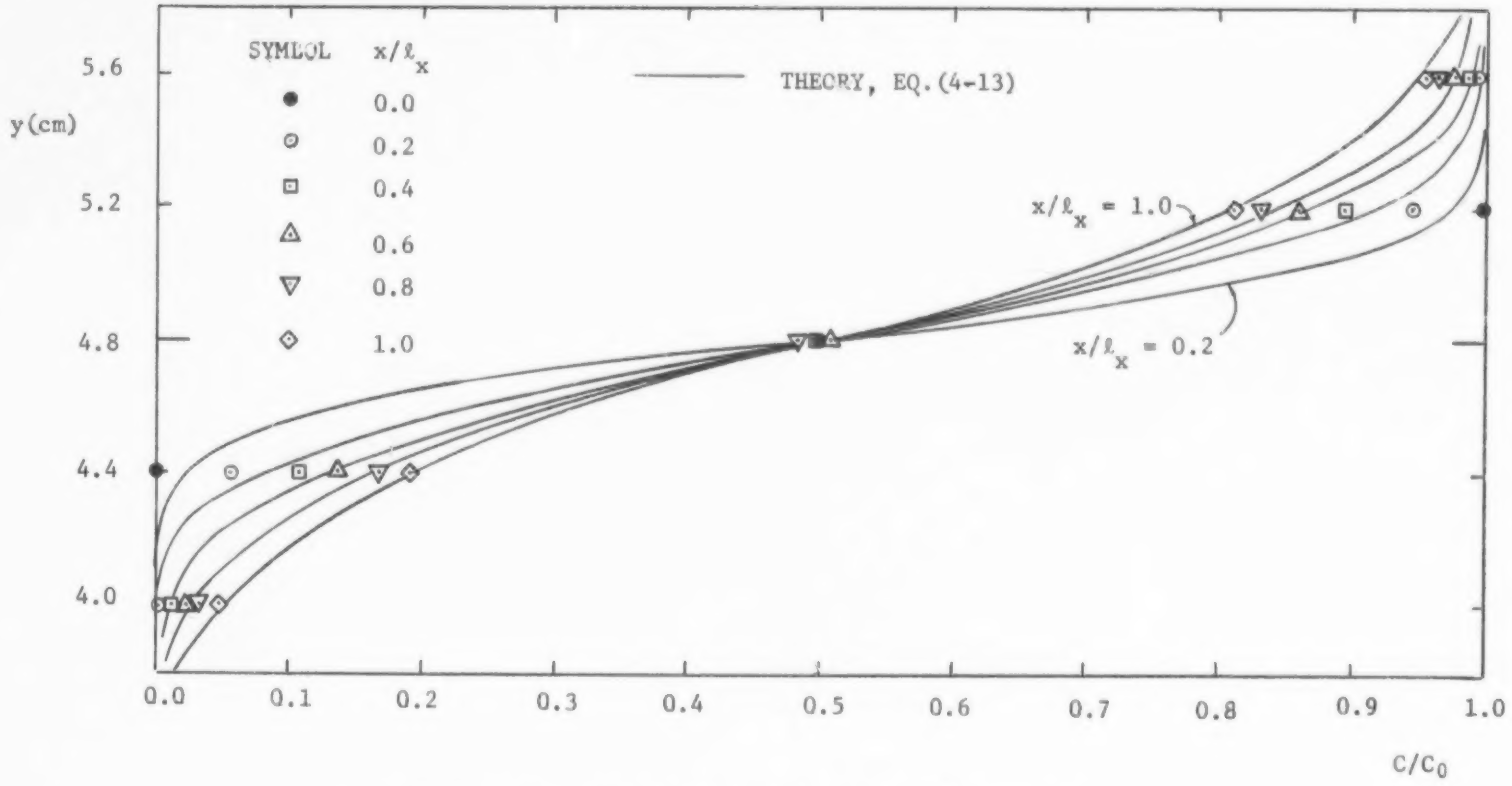


Figure 4-21; Analytical and Numerical Results for Steady State Concentrations, Run T-1

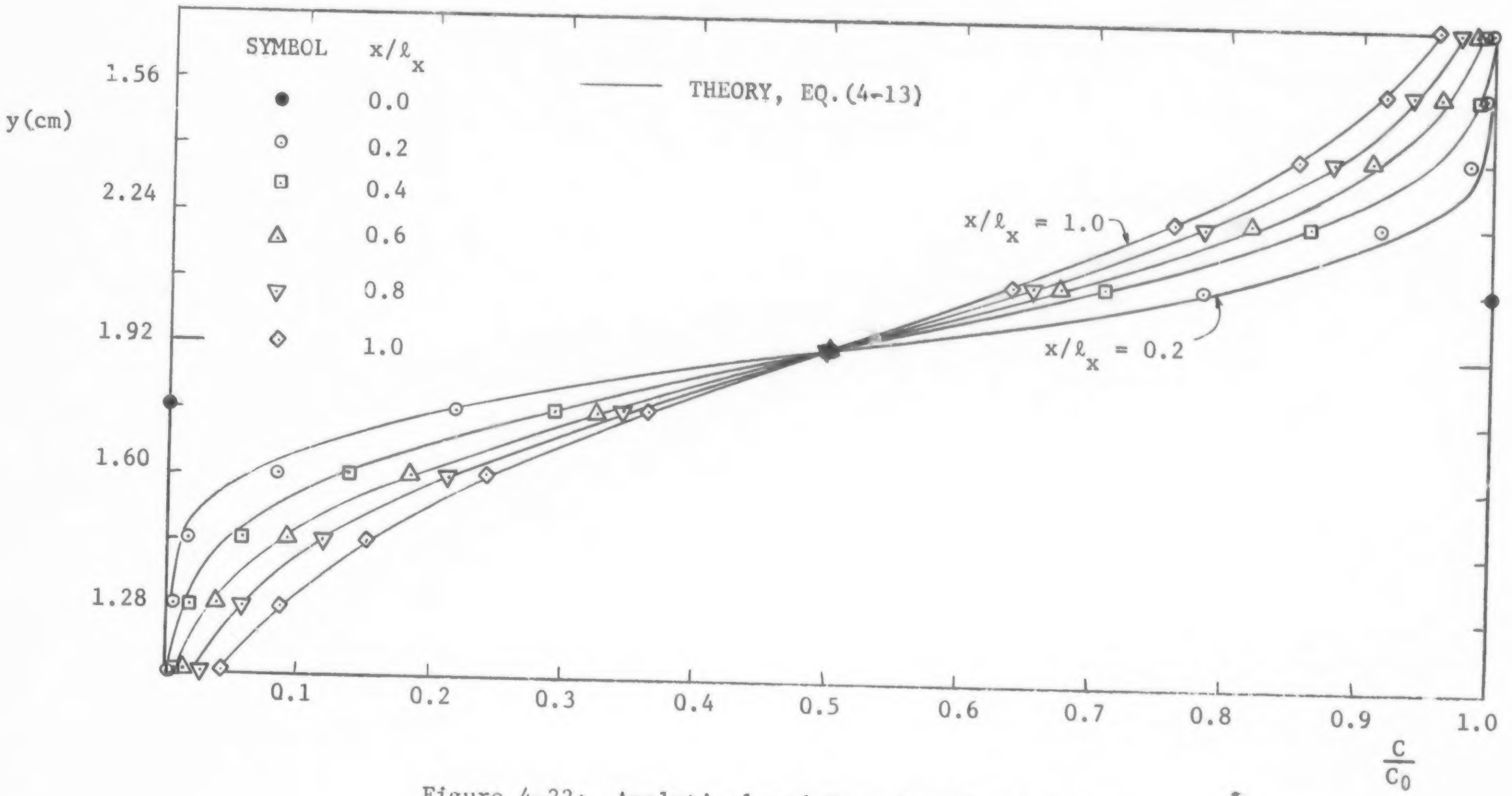


Figure 4-22: Analytical and Numerical Results for Steady State, Run T-2

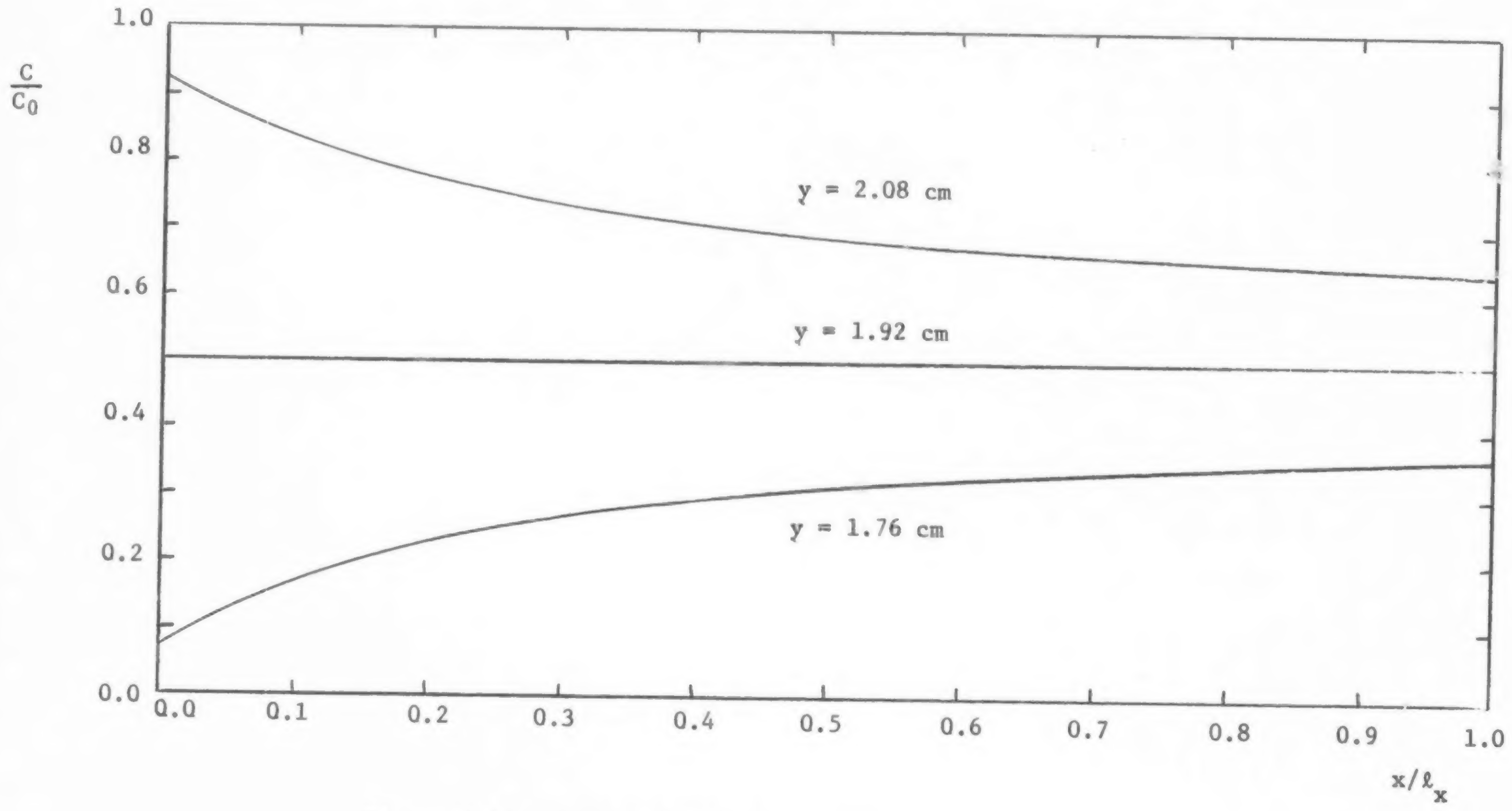


Figure 4-23: Longitudinal Concentration Distribution at Steady State, Run T-2

to the size of the dispersed zone. Another run was made to get better resolution. The data for Run T-2 are the same as for Run T-1 except $0 \leq y \leq 4$ cm and $b = 1.92$ cm. The steady state results are presented in Figure 4-22, and show that the numerical results agree better with equation (4-14) as one proceeds downstream.

Note that the results at steady state are not perfectly symmetrical about the line $y = b$. This is due to the direction of the calculation of the tri-diagonal matrices (from $y = 0$ to $y = \ell_y$). The roundoff error accumulates during the solution of each matrix, and the results at one end of the field are subject to a larger error than at the other. In the present problem the difference is very small. If it is considered too large one may eliminate it by starting the solution at opposite sides on successive time steps.

Figure 4-23 gives the longitudinal concentration distribution at steady state for $y = b + \Delta y = 2.08$ cm, $y = b = 1.92$ cm and $y = b - \Delta y = 1.76$ cm from Run T-2. It is seen that the lines have very small curvature compared with the curves in Figure 4-22. This supports the assumption made by Harleman and Rumer [30], that the longitudinal dispersion term can be neglected for the steady state solution.

4.5 The Two-Well Problem

Hoopes and Harleman [32] have treated a problem of dispersion in the two-dimensional flow field between a recharging and a pumping well which fully penetrates a confined aquifer made of a homogeneous-isotropic porous medium. The flow in the aquifer is due only to the wells, one pumping and the other recharging at an equal constant rate Q, see Figure 4-24.

The source strength is defined by

$$A = \frac{Q}{2\pi b\theta}$$

where θ is the porosity of the media. With this definition the non-dimensional potential is given by

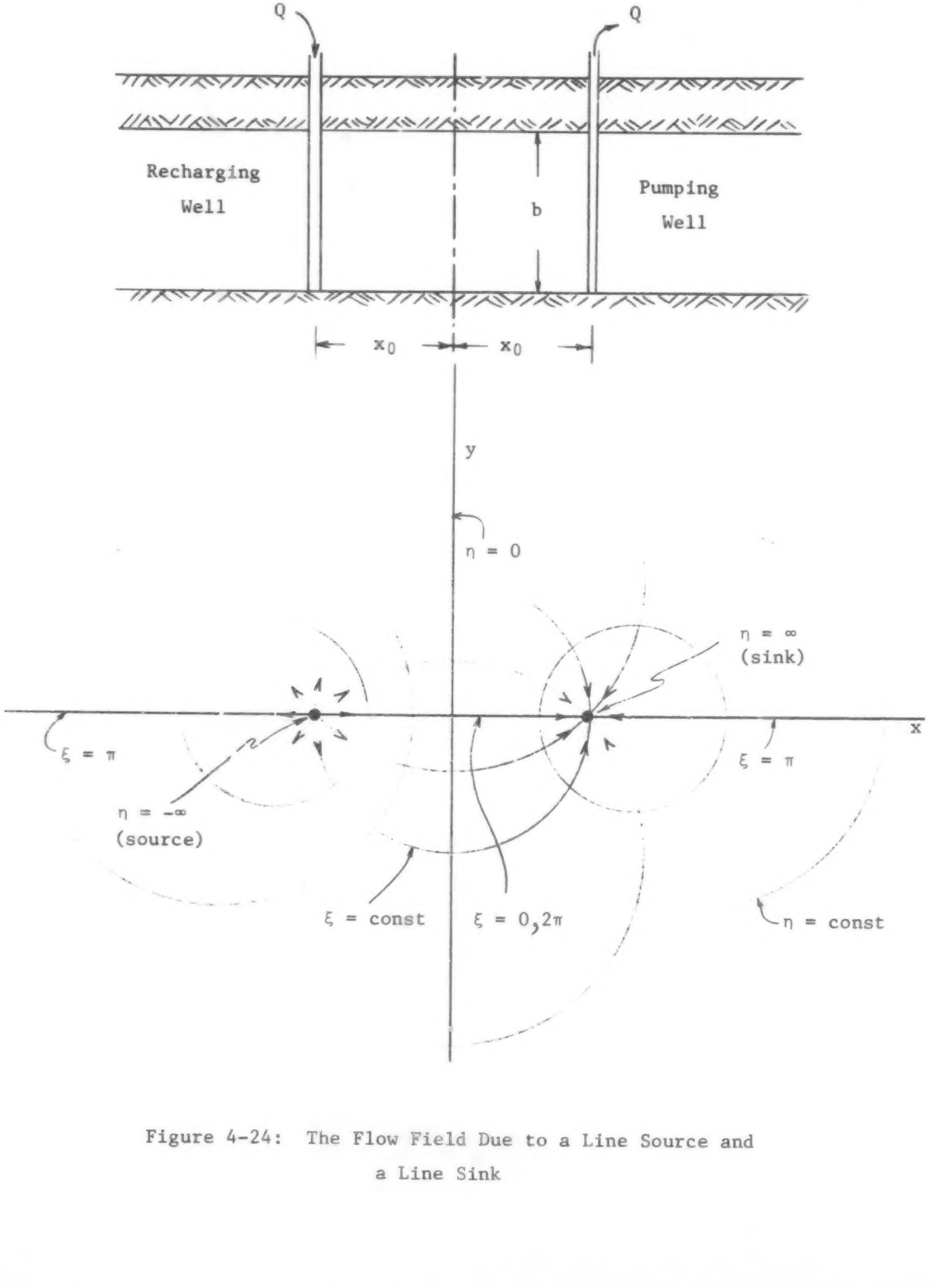

Q
Q
Recharging Well
Pumping Well
b
x_0
x_0
y
$\eta = 0$
$\eta = \infty$ (sink)
x
$\xi = \pi$
$\xi = \pi$
$\eta = -\infty$ (source)
ξ = const
$\xi = 0, 2\pi$
η = const

Figure 4-24: The Flow Field Due to a Line Source and a Line Sink

$$\eta = \frac{\Phi}{A} = \tan^{-1}\left[\frac{2\, x_0\, y}{x_0^2 - (x^2 + y^2)}\right] \qquad (4\text{-}17)$$

and the non-dimensional stream function by

$$\xi = \frac{\psi}{A} = \tanh^{-1}\left[\frac{2\, x_0\, x}{x_0^2 + (x^2 + y^2)}\right] \qquad (4\text{-}18)$$

The non-dimensional velocity along the streamline is given by

$$v = \frac{q\, x_0}{A} = \cosh \eta + \cos \xi \qquad (4\text{-}19)$$

Hoopes and Harleman [32] used the convective dispersion equation in the Φ-ψ coordinates, and considered a step input of concentration at the recharging well. An attempt was made to solve the full equation by an explicit numerical scheme. Due to size limitation on the space and time increments this proved to be an impractical method. Three approximate analytical solutions were found for the simplified equation with:

a. no dispersion, i.e. $\alpha_L = \alpha_T = 0$

b. no lateral dispersion, i.e. $\alpha_T = 0$, $\alpha_L \neq 0$

c. no longitudinal dispersion, i.e. $\alpha_L = 0$, $\alpha_T \neq 0$.

Case (b) was solved numerically for the streamline $\xi = 0, 2\pi$ (the straight line segment between the wells) using an explicit scheme. Nearly 1 hour of IBM 7094 computer time was required to get a solution for this streamline (computed from $\eta = -3.796$ to $\eta = +3.796$). The numerical results for the points ($\eta = 0$, $\xi = 0$) and ($\eta = 3.796$, $\xi = 0$) showed good agreement with the approximate analytical solution for case (b). Results of a few experiments were presented as well.

For the present work the flow field $-4 \leq \eta \leq 4 \quad 0 \leq \xi \leq \pi$ was divided into (25 x 25) equal increments. The full (three equation) scheme was used to compute the concentration distribution in time and space for the whole field. The time step sequence used ($\Delta\tau/\Delta\eta$) from 0.001 to 0.1 with $\Delta\tau$ multiplied by 2.0 at successive time levels. The dispersivity coefficients used were $\alpha_L = 0.15$ and $\alpha_T = 0.0094 (= \alpha_L/16)$, and 1 cycle was

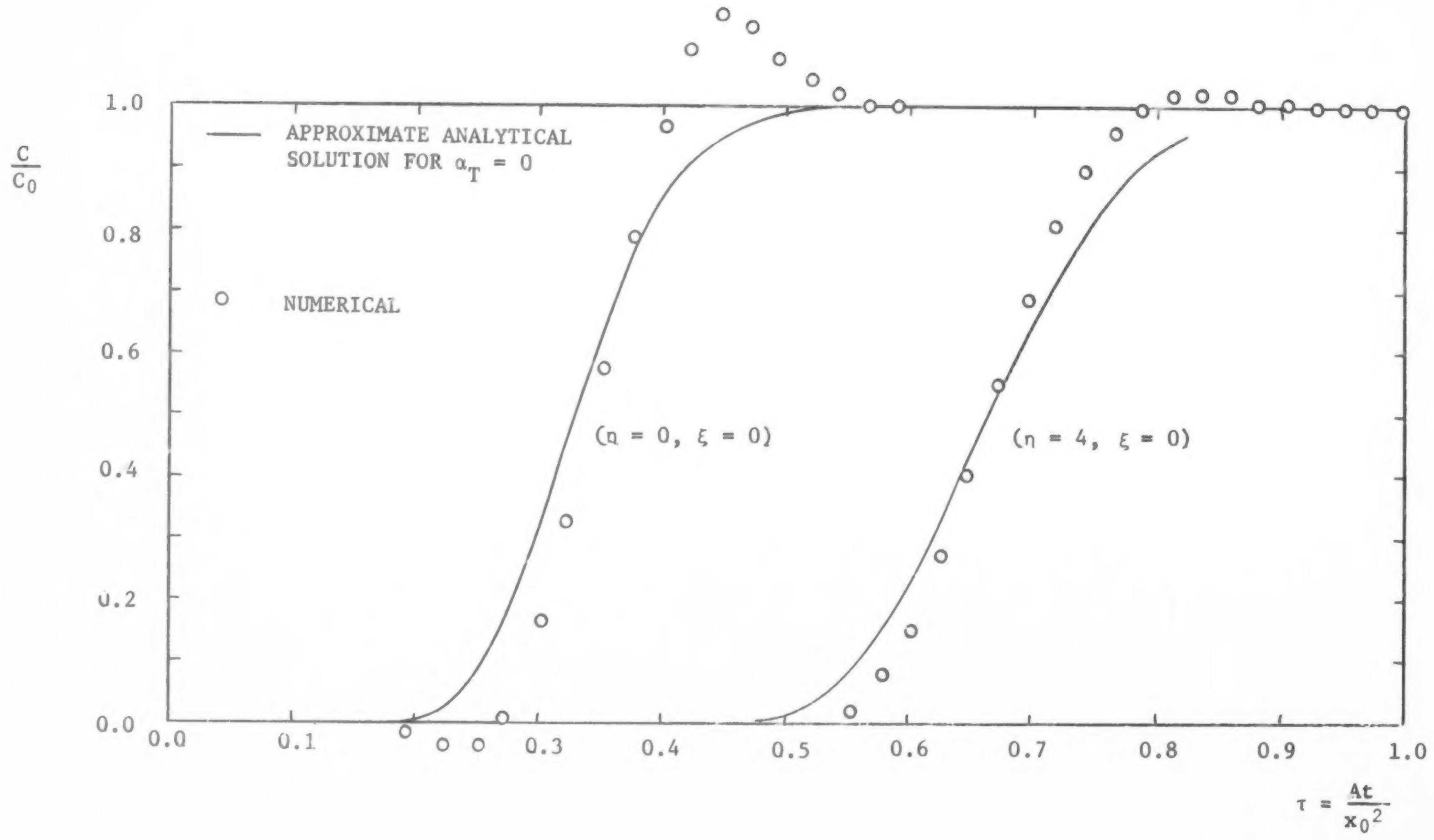


Figure 4-25: The Two Well Problem, Breakthrough Curves at ($\eta = 0$, $\xi = 0$) and ($\eta = 4$, $\xi = 0$)

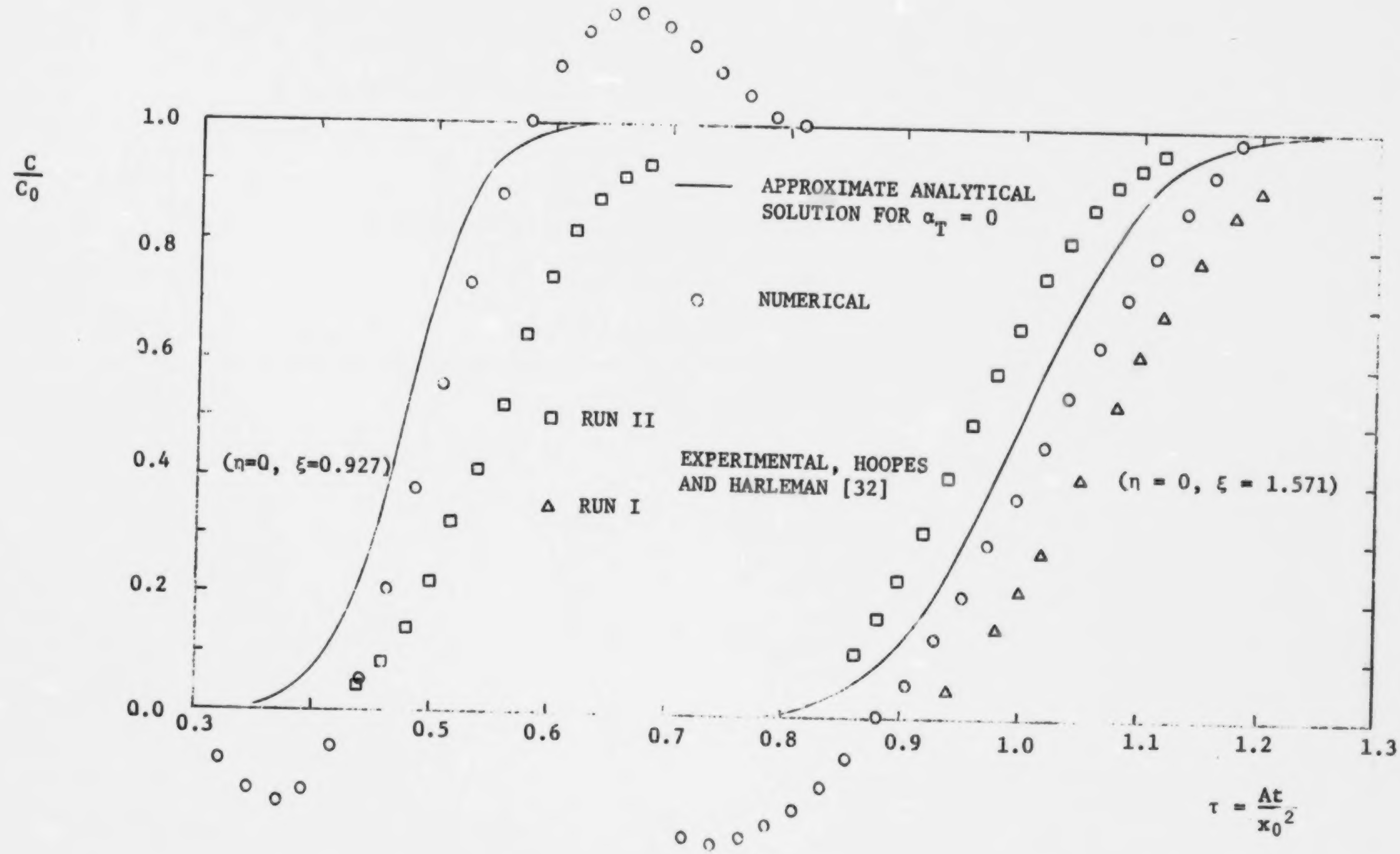


Figure 4-26: The Two Well Problem, Breakthrough Curves at (η = 0, ξ = 0.927) and (η = 0, ξ = 1.571)

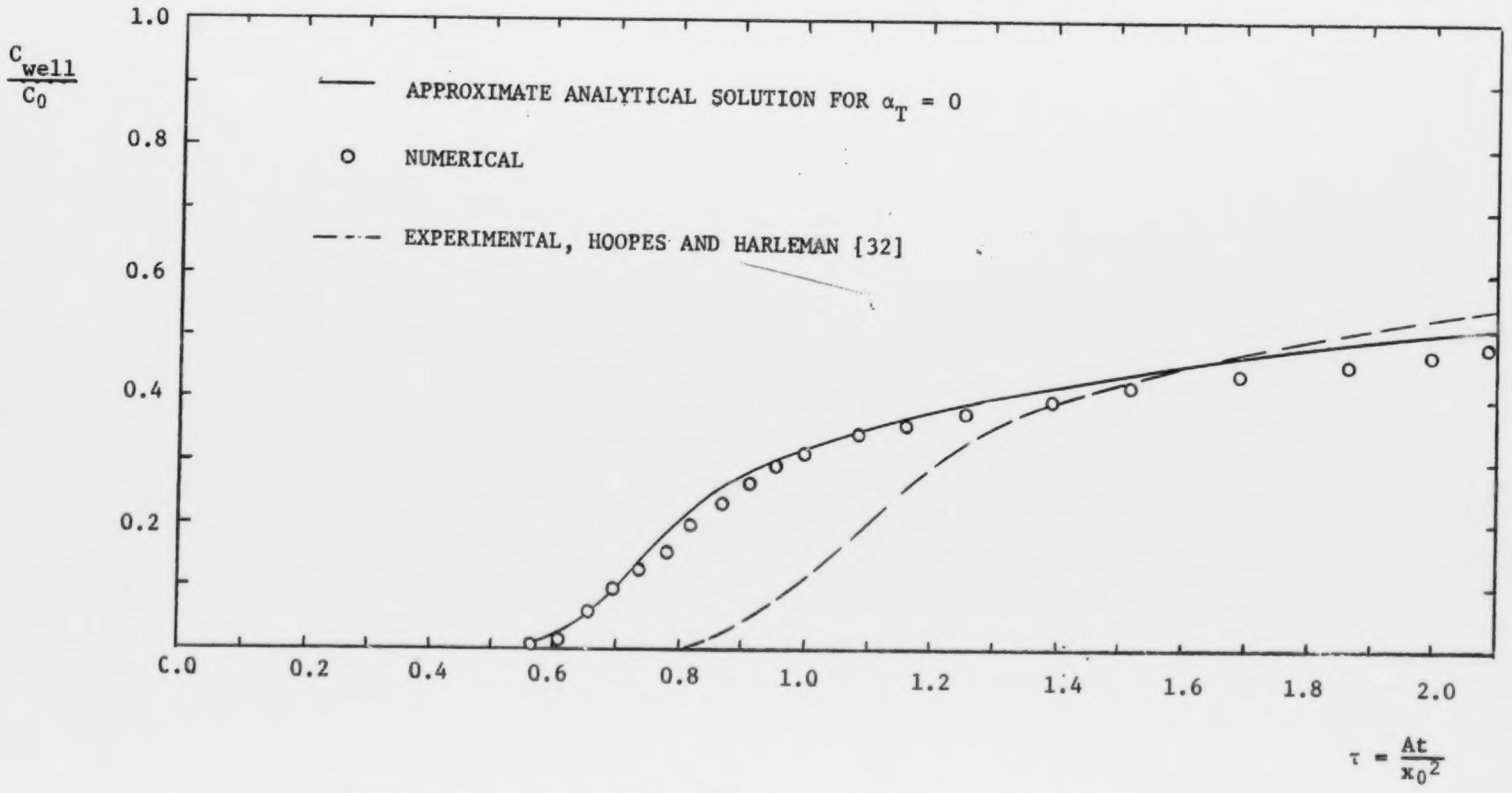


Figure 4-27; The Two Well Problem, Concentration at the Pumping Well used in the η-equation. In 15 minutes of 7094 computer time the solution was carried out to $\tau = 2.13$. At this time the concentration in the pumping well is $0.49\ C_0$, and is increasing very slowly. Results for the points ($\eta = 0$, $\xi = 0$) and ($\eta = 4$, $\xi = 0$) are shown in Figure 4-25. The second point is the end of the streamline $\xi = 0$ close to the pumping well. The approximate analytical solution given by Hoopes and Harleman [32], for the case $\alpha_T = 0$, at the same points is shown in the figure for comparison. The rather large space increments and time step used in the numerical solution for the present work cause the "overshoot" shown. It was not attempted to improve the results by decreasing the space or time increments. Results for the points ($\eta = 0$, $\xi = 0.927$) and ($\eta = 0$, $\xi = 1.571$) are compared with the approximate analytical solution for $\alpha_T = 0$, and with experimental results given by Hoopes and Harleman [32] in Figure 4-26. It is seen that although the numerical results show deviation from the approximate solution, they are in better agreement with it than the experimental results. This is provided the parts where $C < 0$ and $C > C_0$ are discarded as not being physically feasible.

To get the concentration at the pumping well the concentration of all final points on the streamlines was integrated. The results are compared with the prediction of the approximate analytical solution for $\alpha_T = 0$ and with experimental results in Figure 4-27.

The same problem was solved again with $\alpha_T = 0$. For those points in the flow field mentioned above the results were almost identical. The concentration at the pumping well was essentially the same as that shown in Figure 4-26.

This result proves that the assumption $\alpha_T = 0$ does not modify the results for points in the central portion of the flow field.

The two-well problem with a pulse input of length $\tau_c = 0.216$ was also solved numerically for a few streamlines in the field. For these computations α_T was taken to be zero, and the one-equation option was used. The solution was calculated for the streamlines $\xi = 0$ and $\xi = 1.571$ only. Results for a few points are shown in Figures 4-28 and 4-29. The results for the full

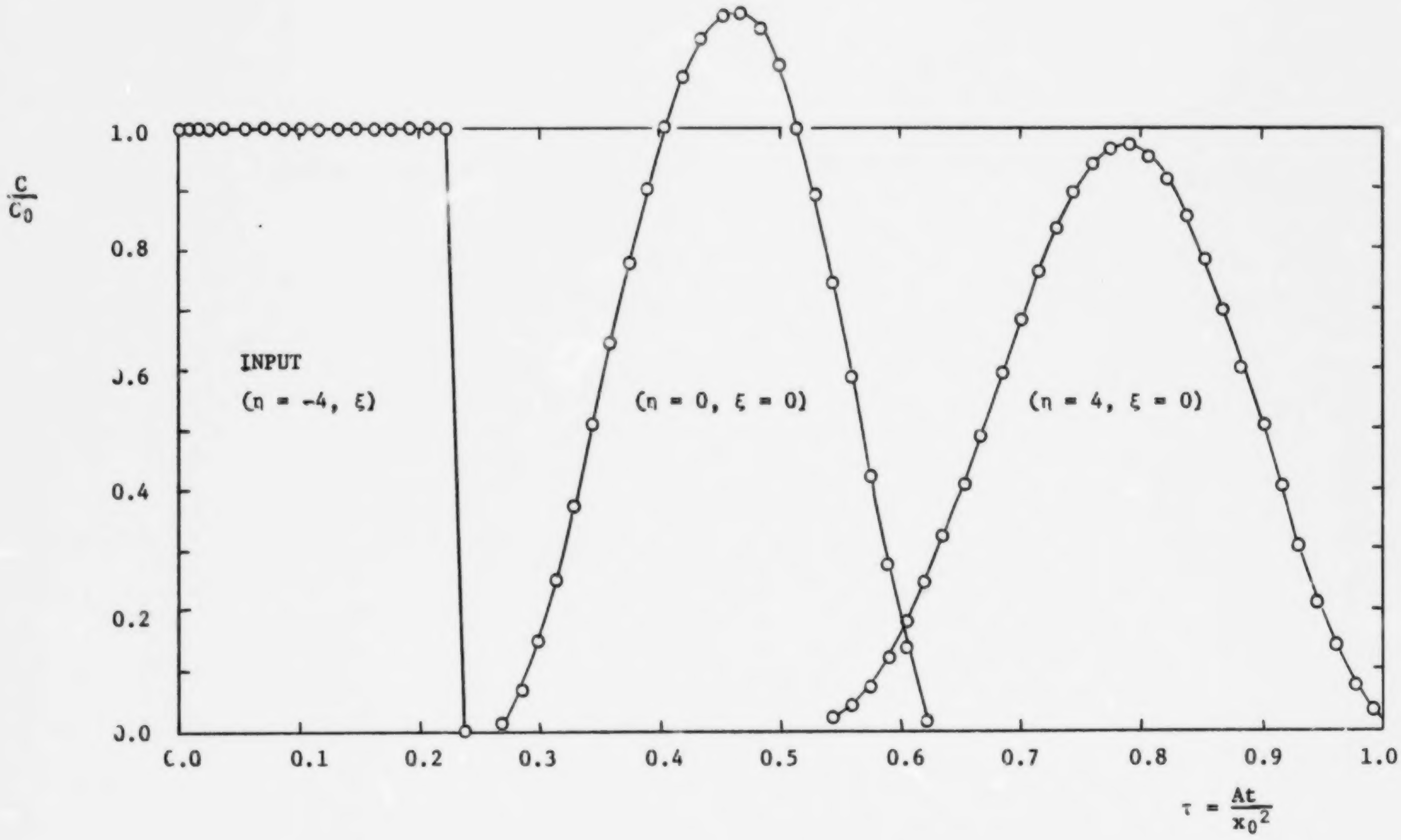


Figure 4-28: The Two Well Problem, Pulse Input, Breakthrough Curves at (η = 0, ξ = 0) and (η = 4, ξ = 0)

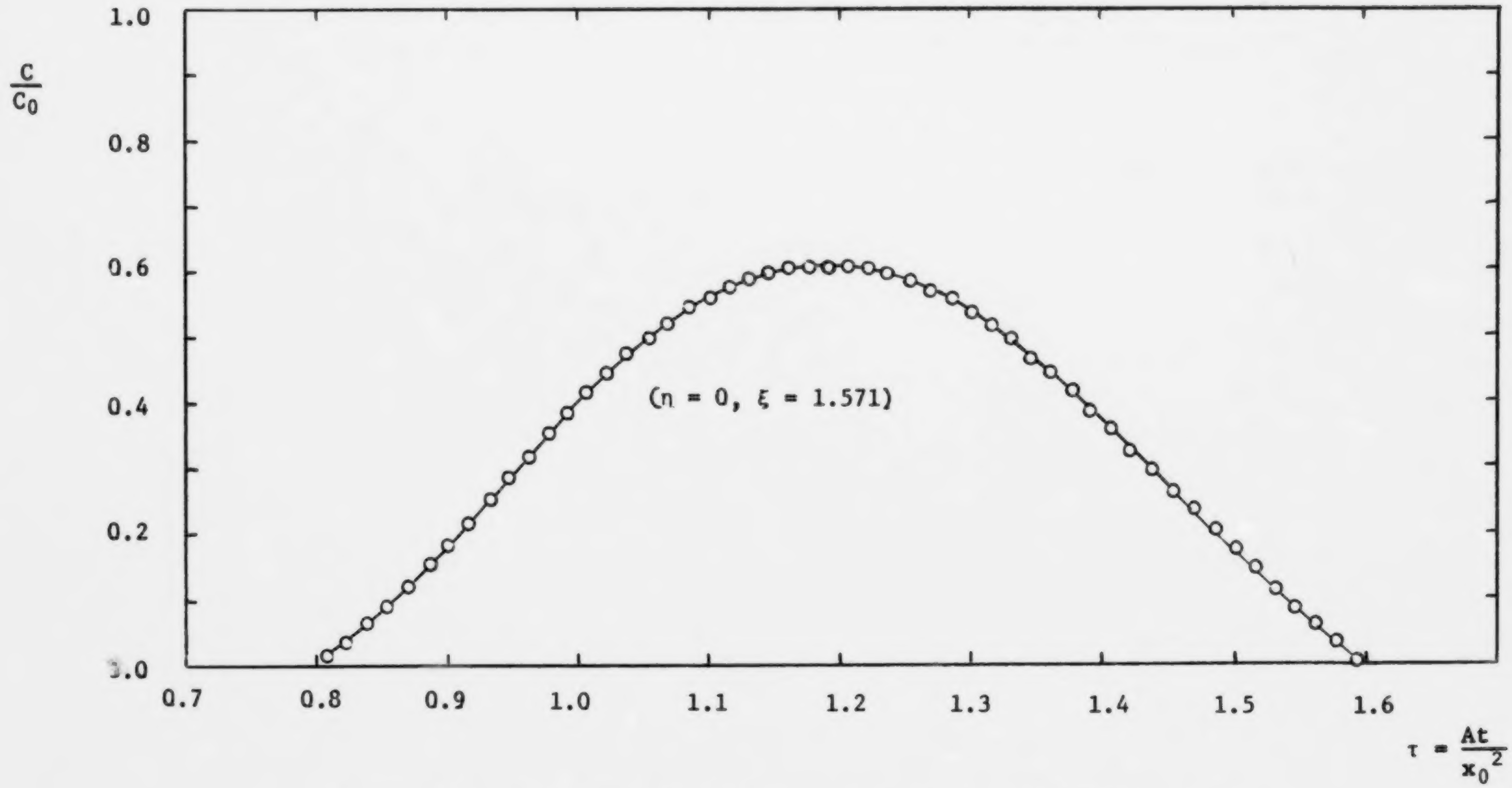


Figure 4-29: The Two Well Problem, Pulse Input, Breakthrough Curve at (η = 0, ξ = 1.571)

length of both these streamlines was computed in 1.8 minutes of computer time for 26 space increments and $(\Delta\tau/\Delta\eta)_{max} = 0.05$.

The two-well problem belongs to the class of problem in which the case of unsteady flow can be solved by the same method, provided the pumping and recharging well have the same temporal variation of Q.

V. DISPERSION IN NON-HOMOGENEOUS POROUS MEDIA

One of the subjects on which very little research has been done is dispersion in non-homogeneous and anisotropic media. Natural aquifers are usually anisotropic and non-homogeneous to some extent. Considering the aquifer as isotropic and homogeneous simplifies the analysis greatly; however this can be done only as a first approximation. The approximation is good for aquifers which are nearly isotropic and in which the scale of non-homogeneity is small (i.e. the size of the homogeneous regions is small and the properties of the media alternate rapidly). When large regions of different materials can be identified, the approximation of the formation by a single homogeneous-isotropic medium may give reasonable results for the concentration distribution at special points in the flow field, but does not describe accurately the whole concentration distribution.

The non-homogeneity considered in this chapter is one of the simplest, but most commonly encountered. The medium is made of layers. Each layer is homogeneous and isotropic, and of uniform thickness. The boundaries between the layers are parallel. For each layer, of given grain size and permeability, there is a unique correlation between the dispersion coefficients and the geometric properties of the medium, the physical properties of the fluid, and the seepage velocity. These correlations will be presented in Section 5.3.1.

The layered medium may also serve as a first approximation to an anisotropic medium. If alternating layers are made of the same material, and the thickness of each layer is small, the formation approximates an anisotropic formation with perpendicular major and minor axes.

The present chapter deals with two problems of dispersion in layered media. The analytical approach and the solutions obtained indicate the methods by which more complex problems might be solved. The analytical solutions also serve as a check for the numerical solutions obtained for these cases.

5.1 Analytical Solutions

5.1.1 Longitudinal Dispersion in a Layered Medium

The problem considered in this section is longitudinal dispersion in a steady unidirectional flow perpendicular to the layers, (Fig. 5-1). The quality of the water flowing through the medium is described by the concentration, C, of some tracer material in solution.

The quality of the inflowing water is changed over the whole cross section as some function of time. A step function will be used, i.e. the concentration is changed instantaneously from zero to some value C_0, and is maintained at this value from this time on.

This "traced" water mixes with the "non-traced" water while flowing through the medium. The mixing causes the sharp concentration interface to be dispersed in the direction of the flow. The amount of dispersion depends on properties of the flow and the medium in which it takes place.

Each layer is homogeneous and isotropic in itself, so the equation describing the convective-dispersion process in the ith layer is

$$\frac{\partial C}{\partial t} + u_i \frac{\partial C}{\partial x_i} = D_{L_i} \frac{\partial^2 C}{\partial x_i^2} \qquad 0 \le x_i \le \ell_i \qquad (5\text{-}1)$$

In this equation adsorption was neglected (see Chapter II), and the lateral dispersion term is not present because there is no concentration gradient in a direction perpendicular to the flow.

When i = 1 in equation (5-1) it applies to the first layer. The boundary conditions for this layer are

$$\begin{aligned} C(x_1,0) &= 0 \qquad & x_1 &\ge 0 \\ C(\infty, t) &= 0 \qquad & t &\ge 0 \end{aligned} \qquad (5\text{-}2)$$

The second condition in (5-2) is the usual one for a homogeneous medium and is valid here although the layer is of finite length.

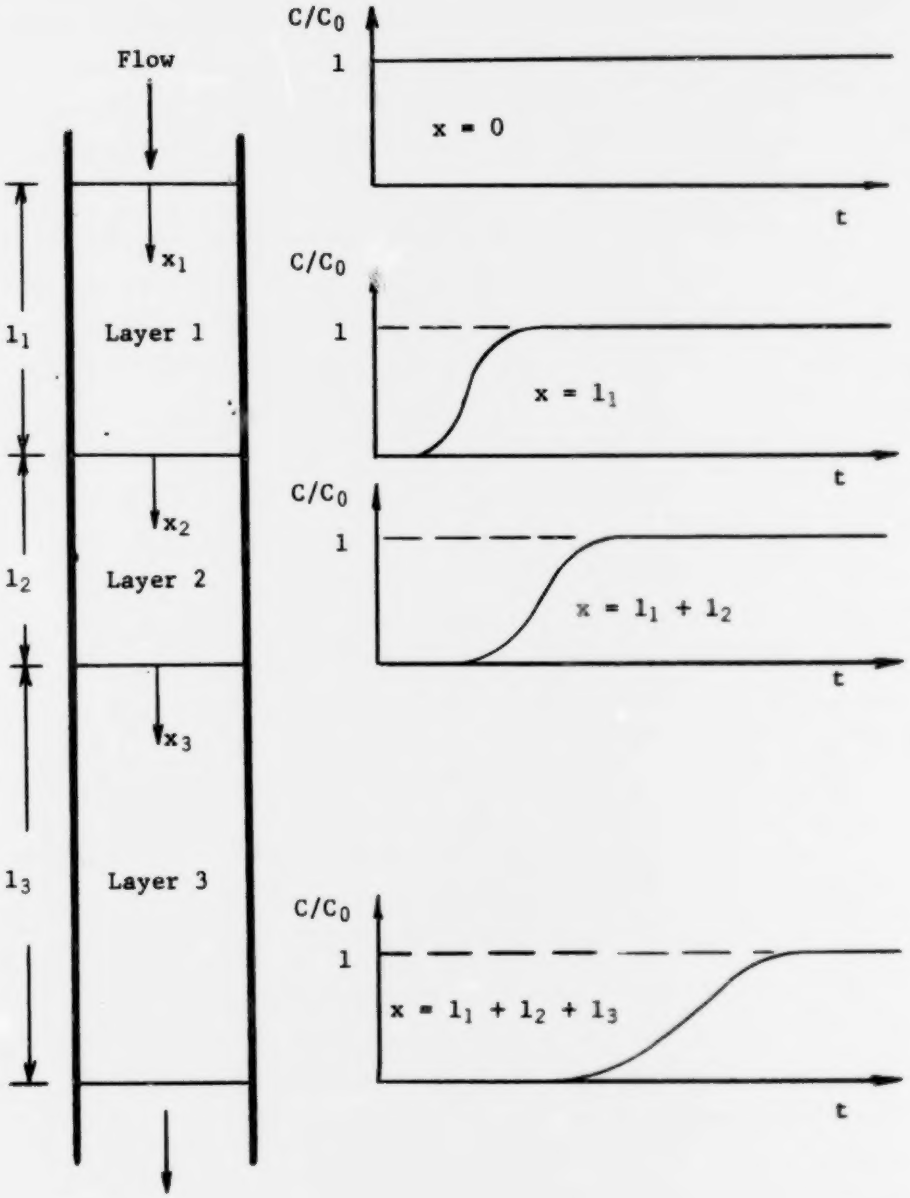

Flow
x_1
Layer 1
l_1
x_2
Layer 2
l_2
x_3
Layer 3
l_3
C/C$_0$
1
x = 0
t
C/C$_0$
1
x = l_1
t
C/C$_0$
1
x = l_1 + l_2
t
C/C$_0$
1
x = l_1 + l_2 + l_3
t

Figure 5-1: Longitudinal Dispersion in Flow Perpendicular to the Layers

The initial condition for the first layer is

$$C(0,t) = C_0 \qquad t \geq 0 \tag{5-3}$$

The concentration distribution in time at the end of the first layer, $x_1 = \ell_1$, is given in terms of the longitudinal dispersion coefficient of the first layer, D_{L_1}, its length, ℓ_1, and the seepage velocity in it, u_1, (Ogata and Banks [39]) by equation (5-4)

$$\frac{C(\ell_1,t)}{C_0} = \frac{1}{2}\,\text{erfc}\left[\frac{\ell_1 - u_1 t}{2\sqrt{D_{L_1} t}}\right] + \frac{1}{2}\exp\left\{\frac{u_1 \ell_1}{D_{L_1}}\right\}\text{erfc}\left[\frac{\ell_1 + u_1 t}{2\sqrt{D_{L_1} t}}\right] \tag{5-4}$$

It has been shown by Ogata and Banks [39], that the second term in equation (5-4) may be neglected when $(D_{L_1}/u_1 \ell_1) < 0.002$ with a maximum possible error of 3%. This condition is usually satisfied under field conditions, and was satisfied in all experiments conducted. A few direct calculations of the second term for experimental conditions showed the error caused by neglecting the second term to be less than 1%.

The concentration at the end of the first layer is then given to a good degree of accuracy by

$$\frac{C(\ell_1,t)}{C_0} = \frac{1}{2}\,\text{erfc}\left[\frac{\ell_1 - u_1 t}{2\sqrt{D_{L_1} t}}\right] \tag{5-5}$$

It will be shown in Section 5.3.1 how equation (5-5) is used in determining the coefficient of longitudinal dispersion of a homogeneous medium from experiments.

The differential equation for the longitudinal dispersion in the second layer is equation (5-1) with $i = 2$. The boundary conditions are as before

$$\begin{aligned} C(x_2,0) &= 0 \qquad & x_2 &\geq 0 \\ C(\infty, t) &= 0 \qquad & t &\geq 0 \end{aligned} \tag{5-6}$$

where $x_2 = 0$ is the beginning of the second layer. The initial condition for layer 2 is the concentration distribution with time at the exit from layer 1, i.e. equation (5-4).

To solve equation (5-1) with the boundary conditions (5-6) and the initial condition (5-4) the Laplace transform is used. The Laplace transform of a function F(t) is defined (Carslaw and Jaeger, [16], p. 298) as

$$L[F(t)] = \bar{F}(p) = \int_{-\infty}^{\infty} F(t)\ e^{-pt}\ dt \tag{5-7}$$

The transformation of equation (5-1), with i = 2, is

$$p\bar{C}(p) + u_2 \frac{d\bar{C}(p)}{dx_2} = D_{L_2} \frac{d^2\bar{C}(p)}{dx_2^2} \tag{5-8}$$

where $\bar{C}(p) = \int_{-\infty}^{\infty} C(t)\ e^{-pt}\ dt.$

The transformed boundary condition is

$$\bar{C}(\infty,p) = 0 \qquad \text{all} \quad p \tag{5-9}$$

and the initial condition (5-4) becomes

$$\bar{C}(0,p) = \frac{C_0}{p} \exp\left\{\left[\frac{u_1 - \sqrt{u_1^2 + 4D_{L_1}p}}{2D_{L_1}}\right]\ell_1\right\} \tag{5-10}$$

The general solution of the ordinary differential equation (5-8) is

$$\bar{C}(x_2,p) = A(p) \exp\left\{\left[\frac{u_2 - \sqrt{u_2^2 + 4D_{L_2}p}}{2D_{L_2}}\right]x_2\right\}$$

$$+ B(p) \exp\left\{\left[\frac{u_2 + \sqrt{u_2^2 + 4D_{L_2}p}}{2D_{L_2}}\right]x_2\right\} \tag{5-11}$$

From equation (5-9) B(p) = 0. Then, using (5-10), we get

$$\bar{C}(0,p) = A(p) = \frac{C_0}{p} \exp \left\{ \left[\frac{u_1 - \sqrt{u_1^2 + 4D_{L_1} p}}{2D_{L_1}} \right] \ell_1 \right\} \qquad (5\text{-}12)$$

The solution of equation (5-8) subject to (5-9) and (5-10) is then

$$\bar{C}(p) = \frac{C_0}{p} \exp \left\{ \left[\frac{u_1 - \sqrt{u_1^2 + 4D_{L_1} p}}{2D_{L_1}} \right] \ell_1 \right\} \cdot$$

$$\cdot \exp \left\{ \left[\frac{u_2 - \sqrt{u_2^2 + 4D_{L_2} p}}{2D_{L_2}} \right] x_2 \right\} \qquad (5\text{-}13)$$

This solution is in the transformed domain. To obtain the solution of equation (5-1) subject to (5-6) and (5-4) one has to get the inverse transform of equation (5-13). This cannot be done directly by the use of tables. The inverse transform may be obtained from its definition (Carslaw and Jaeger, [16], p. 302)

$$F(t) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} \bar{F}(p)\, e^{pt}\, dt \qquad (5\text{-}14)$$

where (a) is taken to the right of any singularities of $\bar{F}(p)$. An alternative method may be used when the transformed equation can be written as a product of two functions, and the inverse transforms of each of these is known.

If $\bar{F}(p) = \bar{g}(p)\cdot\bar{h}(p)$, and if also $g(t)$ and $h(t)$ are known, then the inverse transform of $\bar{F}(p)$ is given by

$$L^{-1}[\bar{F}(p)] = L^{-1}[\bar{g}(p)\cdot\bar{h}(p)] = \int_0^t g(\tau)\cdot h(t-\tau)\, d\tau \qquad (5\text{-}15)$$

The integral appearing in (5-15) is known as the convolution integral (Carslaw and Jaeger, [16], p. 301).

It was decided to use equation (5-15) rather than equation (5-14) to get the inverse transform of equation (5-13) because the results are more readily applicable to the case of more than two layers.

We write equation (5-13) as the product of the two functions of p,

$$\bar{g}(p) = \frac{C_0}{p} \exp \left\{ \left[\frac{u_1 - \sqrt{u_1^2 + 4D_{L_1}p}}{2D_{L_1}} \right] \ell_1 \right\} \tag{5-16}$$

and

$$\bar{h}(p) = \exp \left\{ \left[\frac{u_2 - \sqrt{u_2^2 + 4D_{L_2}p}}{2D_{L_2}} \right] x_2 \right\} \tag{5-17}$$

It is seen that equation (5-16) is identical to equation (5-10), which was the transform of equation (5-4), so that g(t) is given by equation (5-4).

Using Theorem VI § 12.2, and equation (6) in Appendix V of Carslaw and Jaeger [16], the inverse transform of equation (5-17) is

$$h(t) = \frac{x_2}{2\sqrt{\pi D_{L_2} t^3}} \exp\left\{ - \frac{(u_2 t - x_2)^2}{4D_{L_2} t} \right\} \tag{5-18}$$

Then, from equation (5-15) the inverse transform of equation (5-13) is given by

$$C(x_2,t) = \frac{C_0}{2} \int_0^t \left[\operatorname{erfc} \left(\frac{\ell_1 - u_1\tau}{2\sqrt{D_{L_1}\tau}} \right) + \exp\left\{ \frac{u_1\ell_1}{D_{L_1}} \right\} \operatorname{erfc}\left(\frac{\ell_1 + u_1\tau}{2\sqrt{D_{L_1}\tau}} \right) \right] \cdot$$

$$\cdot \left[\frac{x_2}{2\sqrt{\pi D_{L_2}(t - \tau)^3}} \exp\left\{ - \frac{[u_2(t - \tau) - x_2]^2}{4D_{L_2}(t - \tau)} \right\} \right] d\tau \tag{5-19}$$

Equation (5-19) is valid for $0 \le x_2 \le \ell_2$. It gives the concentration distribution in time at a point x_2 in layer 2 after the front has passed through layer 1. At the end of layer 2 the concentration is given by equation (5-19) with $x_2 = \ell_2$.

Equation (5-19) is an exact solution of equation (5-1) with $i = 2$ subject to (5-6) and (5-4). The evaluation of $C(x_2,t)$ for any x_2 must be done numerically, however. To evaluate $C(x_2,t)$ one has to know the seepage velocities u_1 and u_2, the longitudinal dispersion coefficientd D_{L_1} and D_{L_2}, and the lengths ℓ_1 and x_2.

The calculations were carried out by computer. Results are presented in Section 5.3.1.

Equation (5-13) may be written in a different form, which facilitates the extension of the previous results to the case of more than two layers. For $x_2 = \ell_2$ we may write

$$\bar{C}(\ell_2,p) = \frac{C_0}{p} \exp\left\{ \sum_{i=1}^{2} \left[\frac{u_i - \sqrt{u_i^2 + 4D_{L_i}p}}{2D_{L_i}}\right]\ell_i \right\} \tag{5-20}$$

The obvious extension to the case of I layers is

$$\bar{C}(\ell_I,p) = \frac{C_0}{p} \exp\left\{ \sum_{i=1}^{I} \left[\frac{u_i - \sqrt{u_i^2 + 4D_{L_i}p}}{2D_{L_i}}\right]\ell_i \right\} \tag{5-21}$$

Equation (5-21) can again be written as the product of two functions of p. The first includes the summation over the first (I - 1) layers and the second is the term for the Ith layer,

$$\bar{C}(\ell_I,p) = \left[\frac{C_0}{p} \exp\left\{ \sum_{i=1}^{I-1} \left(\frac{u_i - \sqrt{u_i^2 + 4D_{L_i}p}}{2D_{L_i}}\right)\ell_i \right\}\right] \cdot$$

$$\cdot \left[\exp\left\{ \left(\frac{u_I - \sqrt{u_I^2 + 4D_{L_I}p}}{2D_{L_I}}\right)\ell_I \right\}\right] \tag{5-22}$$

Equation (5-22) has now the form $\bar{g}(p)\cdot\bar{h}(p)$, so the inverse is given by the convolution integral, equation (5-15). The inverse of the first part of equation (5-22) is the solution for $C(\ell_{I-1},t)$ found at the end of the (I - 1)st layer. The inverse of the second part is given by equation (5-18) with the subscript 2 replaced by I. The inverse of equation (5-22), which is the solution for $C(\ell_I,t)$

may then be written in the form

$$C(\ell_I,t) = \frac{C_0}{2}\int_0^t C(\ell_{I-1},t)\cdot h(\ell_I;u_I;D_{L_I};t-\tau)d\tau \qquad (5\text{-}23)$$

The method is thus to proceed one layer at a time, use the result for $C(\ell_{I-1},t)$ as $g(t)$ in the convolution with $h(t-\tau)$ from equation (5-18) for the next layer.

To check the validity of this result, and also as a check on the computer program, the following was done. The exact solution for longitudinal dispersion in a homogeneous isotropic medium with $\ell = 40.96$ cm, $D_L = 0.021$ cm^2/sec, and $u = 0.27$ cm/sec was calculated using equation (5-4). Then the length was divided into two, and then three, equal lengths. Each length was considered a "layer", all having the same u and D_L. Equation (5-4) was used for the first layer, and then equation (5-23) was used once for each additional layer.

Figure (5-2) shows the results of this comparison, and it is seen that the agreement is very good. The accuracy of the convolution solution depends on the accuracy with which the numerical integration is performed on the computer. Simpson's rule was used for the integration, and operations were carried out with eight significant figures. The time interval used was 1 second. Due to round-off the error increases with the number of operations. As a result the agreement with the theoretical result is poorer at large times, and the error is larger for three "layers" than for two. It was not attempted to improve the agreement by decreasing the time step in the integration or by using double-precision, in view of the errors in the dispersion coefficients computed from experimental correlations (see Section 5.3.1). The dispersion coefficients used are obtained from experimental correlations, and these include a scatter of the experimental points equivalent to more than 5% uncertainty in the values of D_L.

It is interesting to note from equation (5-21) that

(a) the order of the layers does not affect the final result, and

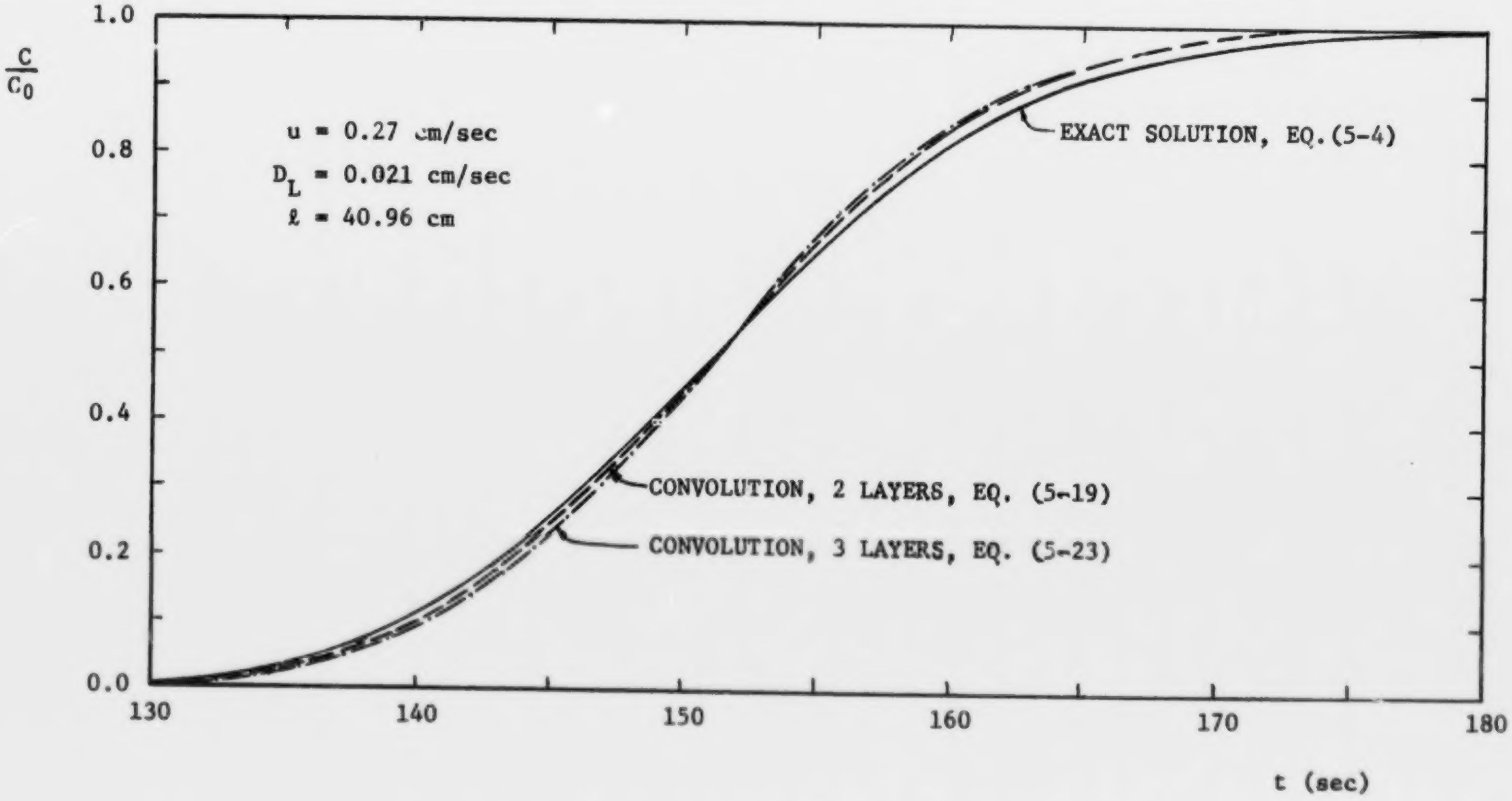


Figure 5-2: Comparison of Exact and Convolution Solutions for a Homogeneous Medium

(b) if the same medium appears in more than one layer one can add up the lengths of the individual layers to one length and use it as a single equivalent layer.

The experimental verification of these results is presented in Section 5.3.2.

5.1.2 Lateral Dispersion in a Layered Medium

We next treat the problem of lateral dispersion in a layered medium with flow along the layers (Fig. 5-3). Each layer is homogeneous and of uniform thickness. The velocity is in the x-direction, which is parallel to the boundaries between the layers, and the flow is steady. The concentration of the fluid entering the medium is a function of the transverse coordinate y. The input concentration considered is a sharp step from zero to C_0 at $y = 0$. The sharp concentration step is dispersed laterally in the downstream direction from the entrance section. The input concentration remains constant and after a sufficiently long time the concentration distribution in the flow field reaches a steady state. This steady state concentration on the cross section $x = x_1$ is denoted by $C(x_1,y)$. The first case considered is that of two layers only. The boundary between the layers is at $y = b_1$. The boundaries of the medium on top and bottom shown in Fig. 5-3 represent the experimental setup, in which the medium was placed in a lucite box (see Section 5.2.3). The width of the layers to these boundaries was made large enough so that the concentration along the lower boundary remains C_0, and along the upper boundary remains zero for all values of x considered. Under these conditions the medium can be thought of as extending to plus and minus infinity for the purpose of analytical treatment.

As the concentration distribution is steady the convective dispersion equation for the ith layer is

$$u_i \frac{\partial C_i}{\partial x} = D_{L_i} \frac{\partial^2 C_i}{\partial x^2} + D_{T_i} \frac{\partial^2 C_i}{\partial y^2} \qquad b_{i-1} \le y \le b_i \qquad (5\text{-}24)$$

where C_i is the concentration in the ith layer, D_{L_i} and D_{T_i} are the coefficients of longitudinal and lateral dispersion, respectively,

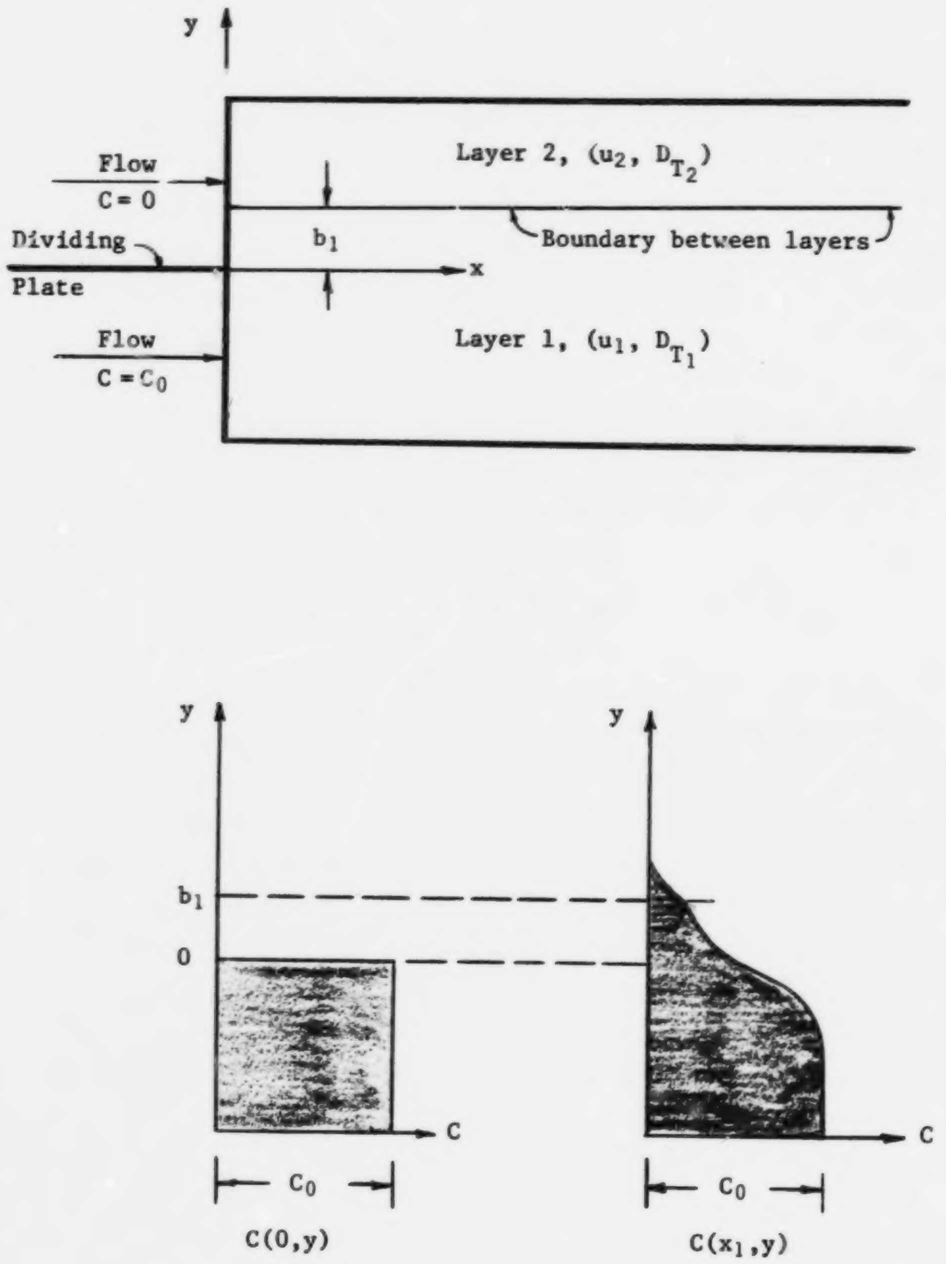

y
Flow
C = 0
Dividing
Plate
Layer 2, (u2, DT2)
b1
Boundary between layers
x
Flow
C = C0
Layer 1, (u1, DT1)
y
b1
0
C
C0
C(0,y)
y
C
C0
C(x1,y)

Figure 5-3: Lateral Dispersion in a Layered Medium with Two Layers

and u_i is the seepage velocity. The ith layer extends from $y = b_{i-1}$ to $y = b_i$.

It has been shown ([28]) that for a homogeneous medium the longitudinal dispersion term in equation (5-24) may be neglected, compared with the other terms. This is because the second derivative of the concentration in the x-direction is a few orders of magnitude smaller than that in the y-direction. Even though $D_L > D_T$ the first product is small. The same assumption is made for the layered medium. Some calculations of the various terms based on experimental results, using finite difference analogues of the derivatives, showed this assumption to be justified.

The reduced equation is then

$$u_i \frac{\partial C_i}{\partial x} = D_{T_i} \frac{\partial^2 C_i}{\partial y^2} \qquad b_{i-1} \le y \le b_i \qquad (5\text{-}25)$$

This equation is written for each layer. In addition to the boundary conditions one has to satisfy compatibility conditions at the layer boundaries. These require equal concentration and equal fluxes in the y-direction across the layer interface, when calculated from the expression for C below and above the boundary. $C(x_1,y)$ has to be continuous at all points but $\partial C(x_1,y)/\partial y$ may have discontinuities at the boundaries.

We use the relation $D_{L_i} = \alpha_{L_i} u_i$ to write for the medium shown in Fig. 5-3

$$\frac{\partial C_1}{\partial x} = \alpha_{L_1} \frac{\partial^2 C_1}{\partial y^2} \qquad -\infty < y \le b_1 \qquad (5\text{-}26)$$

and

$$\frac{\partial C_2}{\partial x} = \alpha_{L_2} \frac{\partial^2 C_2}{\partial y^2} \qquad b_1 \le y < \infty \qquad (5\text{-}27)$$

with the conditions

$$C_1(0,y) = C_0 \qquad -\infty < y < 0 \qquad (5\text{-}28)$$

$$C_1(0,y) = 0 \qquad 0 \le y \le b_i \qquad (5\text{-}29)$$

$$C_0(0,y) = 0 \qquad b_1 \le y < \infty \qquad (5\text{-}30)$$

$$\left.\frac{\partial C_1}{\partial y}\right|_{y\to -\infty} = 0 \quad \text{and} \quad \left.\frac{\partial C_2}{\partial y}\right|_{y\to\infty} = 0 \qquad (5\text{-}31)$$

The compatibility conditions at the interface between the layers are

$$C_1(x,b_1) = C_2(x,b_1) \qquad (5\text{-}32)$$

$$D_{T_1} \left.\frac{\partial C_1}{\partial y}\right|_{y=b_1} = D_{T_2} \left.\frac{\partial C_2}{\partial y}\right|_{y=b_1} \qquad (5\text{-}33)$$

for all x.

To solve equations (5-26) and (5-27) subject to the conditions (5-28) to (5-33) the Laplace transform is used. The transform is made on x, and is defined by

$$L[F(x)] = \bar{F}(p) = \int_0^\infty F(x)\, e^{-px}\, dx \qquad (5\text{-}34)$$

The result of using the Laplace transform is a reduction of the partial differential equation to an ordinary one. The resulting ordinary differential equation incorporates in it the boundary conditions on x = 0. For this reason it is convenient to write three equations, one for medium 2 and one for medium 1 on either side of y = 0. Then these equations are transformed along with their boundary conditions and the compatibility conditions. We write

$$\frac{\partial C_1}{\partial x} = \alpha_{L_1} \frac{\partial^2 C_1}{\partial y^2} \qquad -\infty < y \le 0 \qquad (5\text{-}35)$$

$$\frac{\partial C_1'}{\partial x} = \alpha_{L_1} \frac{\partial^2 C_1'}{\partial y^2} \qquad 0 \le y \le b_1 \qquad (5\text{-}36)$$

$$\frac{\partial C_2}{\partial x} = \alpha_{L_2} \frac{\partial^2 C_2}{\partial y^2} \qquad b_1 \leq y < \infty \qquad (5\text{-}37)$$

A separate equation is written for the parts of medium 1 above and below $y = 0$, but the final expressions for C_1 and C_1' have to be identical.

The conditions on $x = 0$ are

$$C_1(0,y) = C_0 \qquad -\infty < y \leq 0 \qquad (5\text{-}38)$$

$$C_1'(0,y) = 0 \qquad 0 \leq y \leq b_1 \qquad (5\text{-}39)$$

$$C_2(0,y) = 0 \qquad b_1 \leq y < \infty \qquad (5\text{-}40)$$

and the compatibility conditions are

$$C_1(x,0) = C_1'(x,0) \qquad \text{all } x \qquad (5\text{-}41)$$

$$D_{T_1} \left.\frac{\partial C_1}{\partial y}\right|_{y=0} = D_{T_1} \left.\frac{\partial C_1'}{\partial y}\right|_{y=0} \qquad \text{all } x \qquad (5\text{-}42)$$

$$C_1'(x,b_1) = C_2(x,b_1) \qquad \text{all } x \qquad (5\text{-}43)$$

$$D_{T_1} \left.\frac{\partial C_1'}{\partial y}\right|_{y=b_1} = D_{T_2} \left.\frac{\partial C_2}{\partial y}\right|_{y=b_1} \qquad \text{all } x \qquad (5\text{-}44)$$

The transform of equation (5-35) subject to (5-38) is

$$\frac{d^2\bar{C}_1}{dy^2} - q_1^2\,\bar{C}_1 = -\frac{C_0}{\alpha_{L_1}} \qquad -\infty < y \leq 0 \qquad (5\text{-}45)$$

where $q_1^2 = p/\alpha_{L_1}$.

Similarly from equation (5-36)

$$\frac{d^2\bar{C}_1'}{dy^2} - q_1^2\,\bar{C}_1' = 0 \qquad 0 \leq y \leq b_1 \qquad (5\text{-}46)$$

and from equation (5-37)

$$\frac{d^2\bar{C}_2}{dy^2} - q_2^2\,\bar{C}_2 = 0 \qquad b_1 \le y < \infty \qquad (5\text{-}47)$$

where $q_2^2 = p/\alpha_{L_2}$.

The transformed compatibility conditions are

$$\bar{C}_1(0) = \bar{C}_1'(0) \qquad (5\text{-}48)$$

$$\left.\frac{d\bar{C}_1}{dy}\right|_{y=0} = \left.\frac{d\bar{C}_1'}{dy}\right|_{y=0} \qquad (5\text{-}49)$$

$$\bar{C}_1'(b_1) = \bar{C}_2(b_1) \qquad (5\text{-}50)$$

$$D_{T_1}\left.\frac{d\bar{C}_1'}{dy}\right|_{y=b_1} = D_{T_2}\left.\frac{d\bar{C}_2}{dy}\right|_{y=b_1} \qquad (5\text{-}51)$$

The general solution of equation (5-45) is

$$\bar{C}_1 = \frac{C_0}{p} + A_1\,e^{q_1 y} + B_1\,e^{-q_1 y} \qquad -\infty < y \le 0 \qquad (5\text{-}52)$$

For this solution to remain finite as $y \to -\infty$ we must have $B_1 = 0$, then

$$\bar{C}_1 = \frac{C_0}{p} + A_1\,e^{q_1 y} \qquad -\infty < y \le 0 \qquad (5\text{-}53)$$

In a similar manner we get

$$\bar{C}_1' = A_1'\,e^{q_1 y} + B_1'\,e^{-q_1 y} \qquad 0 \le y \le b_1 \qquad (5\text{-}54)$$

and

$$\bar{C}_2 = B_2\,e^{-q_2 y} \qquad b_1 \le y < \infty \qquad (5\text{-}55)$$

From equation (5-48)

$$\frac{C_0}{p} + A_1 = A_1' + B_1' \qquad (5\text{-}56)$$

and from equation (5-49)

$$A_1 = A_1' - B_1' \tag{5-57}$$

Combining, we get

$$B_1' = \frac{C_0}{2p} \tag{5-58}$$

From (5-50)

$$A_1' e^{q_1 b_1} + B_1' e^{-q_1 b_1} = B_2 e^{-q_2 b_1} \tag{5-59}$$

and from (5-51)

$$D_{T_1} q_1 (A_1' e^{q_1 b_1} - B_1' e^{-q_1 b_1}) = - D_{T_2} q_2 B_2 e^{-q_2 b_1} \tag{5-60}$$

Substituting in (5-60) for B_1' from (5-58), and for B_2 from (5-59) gives

$$D_{T_1} q_1 \left(A_1' e^{q_1 b_1} - \frac{C_0}{2p} e^{-q_1 b_1}\right) = - D_{T_2} q_2 \left(A_1' e^{q_1 b_1} + \frac{C_0}{2p} e^{-q_1 b_1}\right) \tag{5-61}$$

which, when solved for A_1', gives

$$A_1' = \frac{C_0}{2p} \left(\frac{1 - L_{21}}{1 + L_{21}}\right) e^{-2q_1 b_1} \tag{5-62}$$

where

$$L_{21} = \sqrt{\frac{D_{T_2} u_2}{D_{T_1} u_1}} = \frac{u_2}{u_1} \sqrt{\frac{\alpha_{T_2}}{\alpha_{T_1}}} \tag{5-63}$$

is a property of both the medium and the flow field. If we use the fact that the gradient in both layers is equal we get

$$L_{21} = \frac{k_2}{k_1} \sqrt{\frac{\alpha_{T_1}}{\alpha_{T_2}}} \tag{5-64}$$

which is a property of the medium only. The notation L_{ij}, given by equation (5-64) will be used from here on.

Solving for A_1 in equation (5-56) yields

$$A_1 = \frac{C_0}{2p}\left[\left(\frac{1 - L_{21}}{1 + L_{21}}\right) e^{-2q_1b_1} - 1\right] \qquad (5\text{-}65)$$

and for B_2 from equation (5-59)

$$B_2 = \frac{C_0}{2p}\left(\frac{1 - L_{21}}{1 + L_{21}}\right) e^{-b_1(q_1 - q_2)} \qquad (5\text{-}66)$$

With these coefficients equations (5-53) to (5-55) become

$$\bar{C}_1 = \frac{C_0}{p} + \frac{C_0}{2p}\left(\frac{1 - L_{21}}{1 + L_{21}}\right) e^{-q_1(2b_1 - y)} - \frac{C_0}{2p} e^{-q_1(-y)}$$

$$- \infty < y \leq 0 \qquad (5\text{-}67)$$

$$\bar{C}_1' = \frac{C_0}{2p}\left(\frac{1 - L_{21}}{1 + L_{21}}\right) e^{-q_1(2b_1 - y)} + \frac{C_0}{2p} e^{-q_1y}$$

$$0 \leq y \leq b_1 \qquad (5\text{-}68)$$

$$\bar{C}_2 = \frac{C_0}{p}\left(\frac{1}{1 + L_{21}}\right) e^{-q_2(y - b_1)-q_1b_1}$$

$$b_1 \leq y < \infty \qquad (5\text{-}69)$$

From a table of transforms (Carslaw and Jaeger, [16], p.494)

$$L\left[\operatorname{erfc} \frac{y}{2\sqrt{\alpha x}}\right] = \frac{e^{-\sqrt{p/\alpha}\, x}}{p} = \frac{e^{-qx}}{p}$$

So the inverse transforms of equation (5-67) can be written directly

$$C_1 = \frac{C_0}{2}\left[2 + \left(\frac{1 - L_{21}}{1 + L_{21}}\right) \operatorname{erfc} \frac{2b_1 - y}{2\sqrt{\alpha_{L_1} x}} - \operatorname{erfc} \frac{(-y)}{2\sqrt{\alpha_{L_1} x}}\right] =$$

$$= \frac{C_0}{2}\left[2 + \left(\frac{1 - L_{21}}{1 + L_{21}}\right) \operatorname{erfc} \frac{2b_1 - y}{2\sqrt{\alpha_{L_1} x}} - \left(1 + \operatorname{erf} \frac{y}{2\sqrt{\alpha_{L_1} x}}\right)\right] =$$

$$= \frac{C_0}{2}\left[\operatorname{erfc}\frac{y}{2\sqrt{\alpha_{L_1}x}} + \left(\frac{1 - L_{21}}{1 + L_{21}}\right)\operatorname{erfc}\frac{2b_1 - y}{2\sqrt{\alpha_{L_1}x}}\right]$$

$$-\infty < y \leq 0 \qquad (5\text{-}70)$$

The transformation of the last term was made keeping in mind that this equation is valid only for $y \leq 0$.

Similarly, from equation (5-68)

$$C_1' = \frac{C_0}{2}\left[\operatorname{erfc}\frac{y}{2\sqrt{\alpha_{L_1}x}} + \left(\frac{1 - L_{21}}{1 + L_{21}}\right)\operatorname{erfc}\frac{2b_1 - y}{2\sqrt{\alpha_{L_1}x}}\right]$$

$$0 \leq y \leq b_1 \qquad (5\text{-}71)$$

which is seen to be identical to (5-70). From (5-69),

$$C_2 = \frac{C_0}{1 + L_{21}}\operatorname{erfc}\left[\frac{(y - b_1)\sqrt{\alpha_{L_1}} + b_1\sqrt{\alpha_{L_2}}}{2\sqrt{\alpha_{L_1}\alpha_{L_2}x}}\right]$$

$$b_1 \leq y < \infty \qquad (5\text{-}72)$$

Equations (5-70) and (5-72) give the solution in medium 1 and 2 respectively. Conditions (5-48) and (5-49) are satisfied automatically, by the identity of equations (5-70) and (5-71). The conditions (5-50) and (5-51) are satisfied, as can be verified directly.

The validity of the solution can be checked in two ways:

a. For a homogeneous medium $L_{21} = 1$, $b_1 = 0$ and $\alpha_{L_1} = \alpha_{L_2} = \alpha_L$, then

$$C_1 = \frac{C_0}{2}\operatorname{erfc}\left[\frac{y}{2\sqrt{\alpha_L x}}\right] \qquad -\infty < y \leq 0$$

$$(5\text{-}73)$$

$$C_2 = \frac{C_0}{2}\operatorname{erfc}\left[\frac{y}{2\sqrt{\alpha_L x}}\right] \qquad 0 \leq y < \infty$$

which is the known solution for a homogeneous medium ([28]).

b. For $b_1 = 0$ the solution is given in Carslaw and Jaeger [16], p. 88. Equations (5-70) and (5-72) can be reduced to the form given there when $b_1 = 0$.

The method presented for two layers is applicable to the case of more than two, as outlined briefly for the case of three layers, shown in Fig. 5-4.

The differential equations are:

$$\frac{\partial C_1}{\partial x} = \alpha_{L_1} \frac{\partial^2 C_1}{\partial y^2} \qquad -\infty < y < 0 \qquad (5\text{-}74)$$

$$\frac{\partial C_1'}{\partial x} = \alpha_{L_1} \frac{\partial^2 C_1'}{\partial y^2} \qquad 0 \le y < b_1 \qquad (5\text{-}75)$$

$$\frac{\partial C_2}{\partial x} = \alpha_{L_2} \frac{\partial^2 C_2}{\partial y^2} \qquad b_1 \le y < b_2 \qquad (5\text{-}76)$$

$$\frac{\partial C_3}{\partial x} = \alpha_{L_3} \frac{\partial^2 C_3}{\partial y^2} \qquad b_2 \le y < \infty \qquad (5\text{-}77)$$

with the boundary conditions

$$C_1(0,y) = C_0 \qquad -\infty < y < 0 \qquad (5\text{-}78)$$

$$C_1'(0,y) = 0 \qquad 0 \le y < b_1 \qquad (5\text{-}79)$$

$$C_2(0,y) = 0 \qquad b_1 \le y < b_2 \qquad (5\text{-}80)$$

$$C_3(0,y) = 0 \qquad b_2 \le y < \infty \qquad (5\text{-}81)$$

The compatibility conditions are

$$C_1(x,0) = C_1'(x,0) \qquad (5\text{-}82)$$

$$\left.\frac{\partial C_1}{\partial y}\right|_{y=0} = \left.\frac{\partial C_1'}{\partial y}\right|_{y=0} \qquad (5\text{-}83)$$

$$C_1'(x,b_1) = C_2(x,b_1) \qquad (5\text{-}84)$$

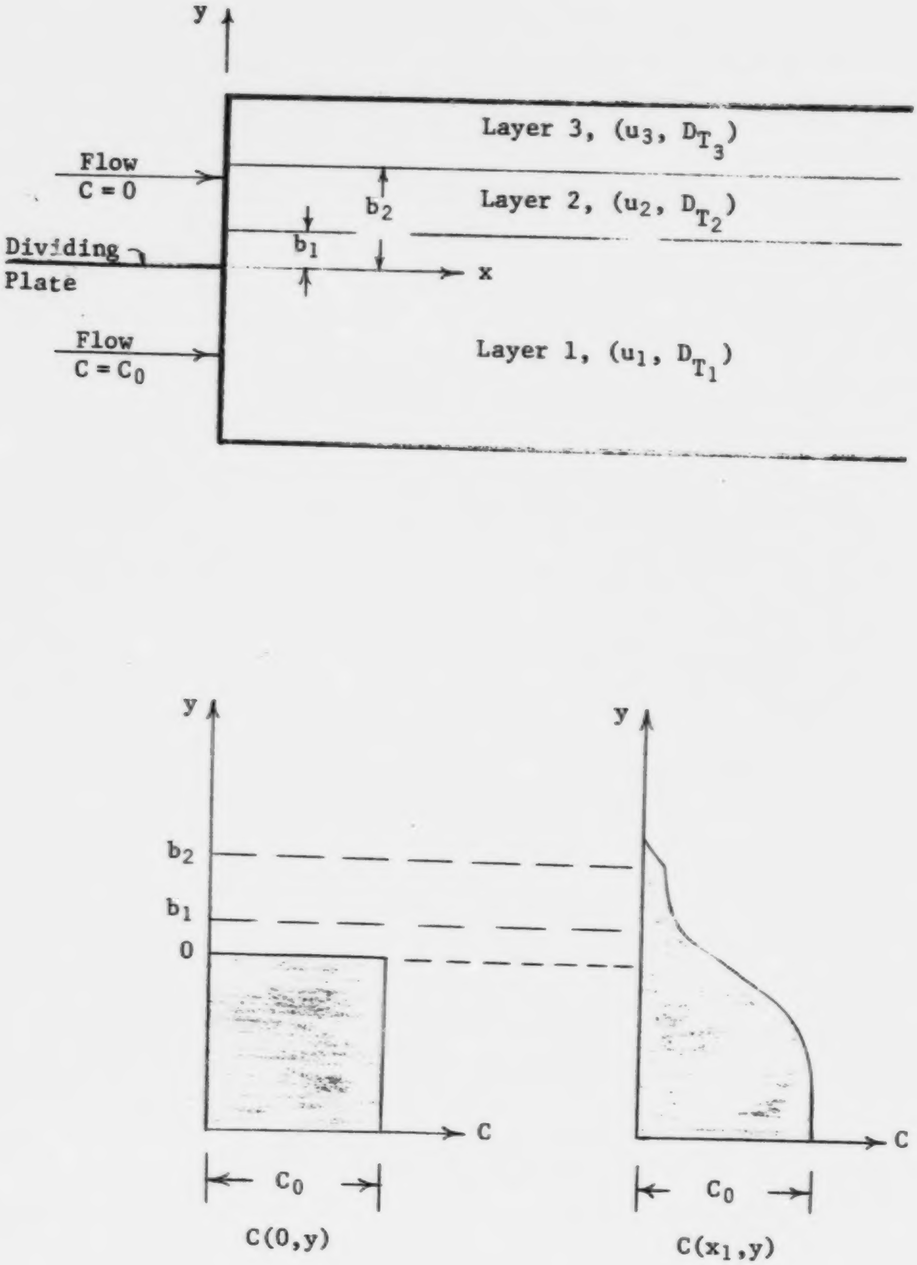

y
Layer 3, (u_3, D_{T_3})
Flow
C = 0
b_2
Layer 2, (u_2, D_{T_2})
b_1
Dividing
Plate
x
Flow
C = C_0
Layer 1, (u_1, D_{T_1})
y
b_2
b_1
0
C
C_0
C(0,y)
y
C
C_0
C(x_1,y)

Figure 5-4: Lateral Dispersion in a Layered Medium with Three Layers

$$D_{T_1} \left.\frac{\partial C_1'}{\partial y}\right|_{y=b_1} = D_{T_2} \left.\frac{\partial C_2}{\partial y}\right|_{y=b_1} \tag{5-85}$$

$$C_2(x,b_2) = C_3(x,b_2) \tag{5-86}$$

$$D_{T_2} \left.\frac{\partial C_2}{\partial y}\right|_{y=b_2} = D_{T_3} \left.\frac{\partial C_3}{\partial y}\right|_{y=b_2} \tag{5-87}$$

When the equations (5-74) to (5-77) are transformed we get a set of equations similar to equations (5-45) to (5-47), where only the one resulting from equation (5-74) has a non-zero right hand side. The general solutions of the transformed equations are found as before. Then the transforms of conditions (5-82) to (5-87) are used to determine the coefficients. The resulting transformed equation of (5-74) is

$$\begin{aligned}\bar{C}_1 = \frac{C_0}{p} + \frac{C_0}{2p} \Bigg[& \left(\frac{1 - L_{21}}{1 + L_{31}}\right) \exp\{- q_1(2b_1 - y)\} + \\ & + \left(\frac{L_{21} - L_{31}}{1 + L_{31}}\right) \exp\{- q_2(- 2b_2 - 2b_1) - q_1(b_1 - y)\} - \\ & - \exp\{- q_1(- y)\}\Bigg]\end{aligned} \tag{5-88}$$

The inverse is

$$\begin{aligned}C_1 = C_0 + \frac{C_0}{2} \Bigg[& \left(\frac{1 - L_{21}}{1 + L_{31}}\right. \operatorname{erfc}\left(\frac{2b_1 - y}{2\sqrt{\alpha_{L_1} x}}\right) + \left(\frac{L_{21} - L_{31}}{1 + L_{31}}\right) \operatorname{erfc} \\ & \left(\frac{(b_1 - y)\sqrt{\alpha_{L_2}} - 2(b_1 + b_2)\sqrt{\alpha_{L_1}}}{2\sqrt{\alpha_{L_1}\alpha_{L_2} x}}\right) - \operatorname{erfc} \left.\frac{- y}{2\sqrt{\alpha_{L_1} x}}\right)\Bigg] = \\ = \frac{C_0}{2} \Bigg[& \operatorname{erfc}\left(\frac{y}{2\sqrt{\alpha_{L_1} x}}\right) + \left(\frac{1 - L_{21}}{1 + L_{31}}\right) \operatorname{erfc}\left(\frac{2b_1 - y}{2\sqrt{\alpha_{L_1} x}}\right) \\ & + \left(\frac{L_{21} - L_{31}}{1 + L_{31}}\right) \operatorname{erfc}\left(\frac{(b_1 - y)\sqrt{\alpha_{L_2}} - 2(b_1 + b_2)\sqrt{\alpha_{L_1}}}{2\sqrt{\alpha_{L_1}\alpha_{L_2} x}}\right)\Bigg]\end{aligned}$$

$$- \infty < y < 0 \tag{5-89}$$

The solution of the transform of (5-75) is

$$\bar{C}_1' = \frac{C_0}{2p}\left[\left(\frac{1 - L_{21}}{1 + L_{31}}\right) \exp\left\{- q_1(2b_1 - y)\right\} + \left(\frac{L_{21} - L_{31}}{1 + L_{31}}\right)\right.$$

$$\left. \exp\left\{ - q_2(- 2b_2 - 2b_1) - q_1(b_1 - y)\right\} + \exp\left\{- q_1 y\right\}\right] \qquad (5\text{-}90)$$

The inverse of (5-90) is

$$C_1' = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{y}{2\sqrt{\alpha_{L_1} x}}\right) + \left(\frac{1 - L_{21}}{1 + L_{31}}\right) \operatorname{erfc}\left(\frac{2b_1 - y}{2\sqrt{\alpha_{L_1} x}}\right)\right.$$

$$\left. + \left(\frac{L_{21} - L_{31}}{1 + L_{31}}\right) \operatorname{erfc}\left(\frac{(b_1 - y)\sqrt{\alpha_{L_2}} - 2(b_1 + b_2)\sqrt{\alpha_{L_1}}}{2\sqrt{\alpha_{L_1}\alpha_{L_2} x}}\right)\right]$$

$$0 \le y < b_1 \qquad (5\text{-}91)$$

which is identical with equation (5-89). The solution of the transform of (5-76) is

$$\bar{C}_2 = \frac{C_0}{2p}\left[\left(\frac{1 - L_{32}}{1 + L_{31}}\right) \exp\left\{- q_2(2b_2 - b_1 - y) - q_1 b_1\right\}\right.$$

$$\left. + \left(\frac{1 + L_{32}}{1 + L_{31}}\right) \exp\left\{- q_2(b_1 - y) - q_1 b_1\right\}\right] \qquad (5\text{-}92)$$

and the inverse transform is

$$C_2 = \frac{C_0}{2}\left[\left(\frac{1 - L_{32}}{1 + L_{31}}\right) \operatorname{erfc}\left(\frac{(2b_2 - b_1 - y)\sqrt{\alpha_{L_1}} + b_1\sqrt{\alpha_{L_2}}}{2\sqrt{\alpha_{L_1}\alpha_{L_2} x}}\right)\right.$$

$$\left. + \left(\frac{1 + L_{32}}{1 + L_{31}}\right) \operatorname{erfc}\left(\frac{(b_1 - y)\sqrt{\alpha_{L_1}} - b_1\sqrt{\alpha_{L_2}}}{2\sqrt{\alpha_{L_1}\alpha_{L_2} x}}\right)\right]$$

$$b_1 \le y < b_2 \qquad (5\text{-}93)$$

The transformed solution for (5-77) is

$$\bar{C}_3 = \frac{C_0}{p}\left[\left(\frac{1}{1 + L_{31}}\right) \exp\left\{- q_3(y - b_2) - q_2(b_2 - b_1) - q_1 b_1\right\}\right] \tag{5-94}$$

for which the inverse transformation gives

$$C_3 = \frac{C_0}{1 + L_{31}} \operatorname{erfc}\left(\frac{(y - b_2)\sqrt{\alpha_{L_1}\alpha_{L_2}} + (b_2 - b_1)\sqrt{\alpha_{L_1}\alpha_{L_3}} + b_1\sqrt{\alpha_{L_2}\alpha_{L_3}}}{2\sqrt{\alpha_{L_1}\alpha_{L_2}\alpha_{L_3} x}}\right)$$

$$b_2 \le y < \infty \tag{5-95}$$

To check the validity this is reduced to the case of two layers with $b_1 = b_2$, $L_{32} = 1$, $L_{31} = L_{21}$, $\alpha_{L_3} = \alpha_{L_2}$. For C_1 and C_2 the equations

$$C_1 = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{y}{2\sqrt{\alpha_{L_1} x}}\right) + \left(\frac{1 - L_{21}}{1 + L_{21}}\right) \operatorname{erfc}\left(\frac{2b_1 - y}{2\sqrt{\alpha_{L_1} x}}\right)\right]$$

$$- \infty < y < b_1 \tag{5-96}$$

and

$$C_2 = \frac{C_0}{1 + L_{21}} \operatorname{erfc}\left(\frac{(y - b_1)\sqrt{\alpha_{L_1}} + b_1\sqrt{\alpha_{L_2}}}{2\sqrt{\alpha_{L_1}\alpha_{L_2} x}}\right)$$

$$b_1 \le y < \infty \tag{5-97}$$

are obtained, which are the same as equations (5-70) and (5-72).

The extension of the above results to the case of more layers is not obvious. Only the equation for the uppermost layer can be written in a general form. However the analysis indicates the method to be employed for all similar cases, e.g. when there are more layers below $y = 0$.

5.2 Experimental Equipment and Procedures

5.2.1 Measurement of Concentration

The tracer used in the experiments was Sodium Chloride (NaCl) with a maximum concentration of 0.2% by weight. The property used to determine the concentration of a salt solution in water is its electrical conductivity. The relation between concentration and conductance is nearly linear. A sample plot of conductance vs. concentration is shown in Fig. 5-5, for concentrations of 0% to 0.05%. For a constant temperature, and over a small enough range of concentrations this relation can be written

$$\gamma = \beta C \tag{5-98}$$

where γ = specific conductance of the solution, mhos/cm

C = concentration, ppm

β = a temperature dependent coefficient.

For best accuracy in determining C from γ one should use curves such as Fig. 5-5 (data is given in Handbook of Chemistry and Physics [27] and in International Critical Tables). As conductance is very sensitive to temperature changes, one has to measure the temperature accurately in order to be able to convert conductance to concentration.

When one is interested in a relative change in concentration, and not the actual concentration, and if one can consider β to be a constant over the range of concentrations C_{min} to C_{max}, then

$$\frac{C - C_{min}}{C_{max} - C_{min}} = \frac{\gamma - \gamma_{min}}{\gamma_{max} - \gamma_{min}} \tag{5-99}$$

which is independent of β.

When samples were taken their concentration was measured using a conductivity bridge (Type RC by Industrial Instruments, Inc.). All samples were at the same temperature and the range of concentrations was small, so equation (5-99) was used to determine relative concentration.

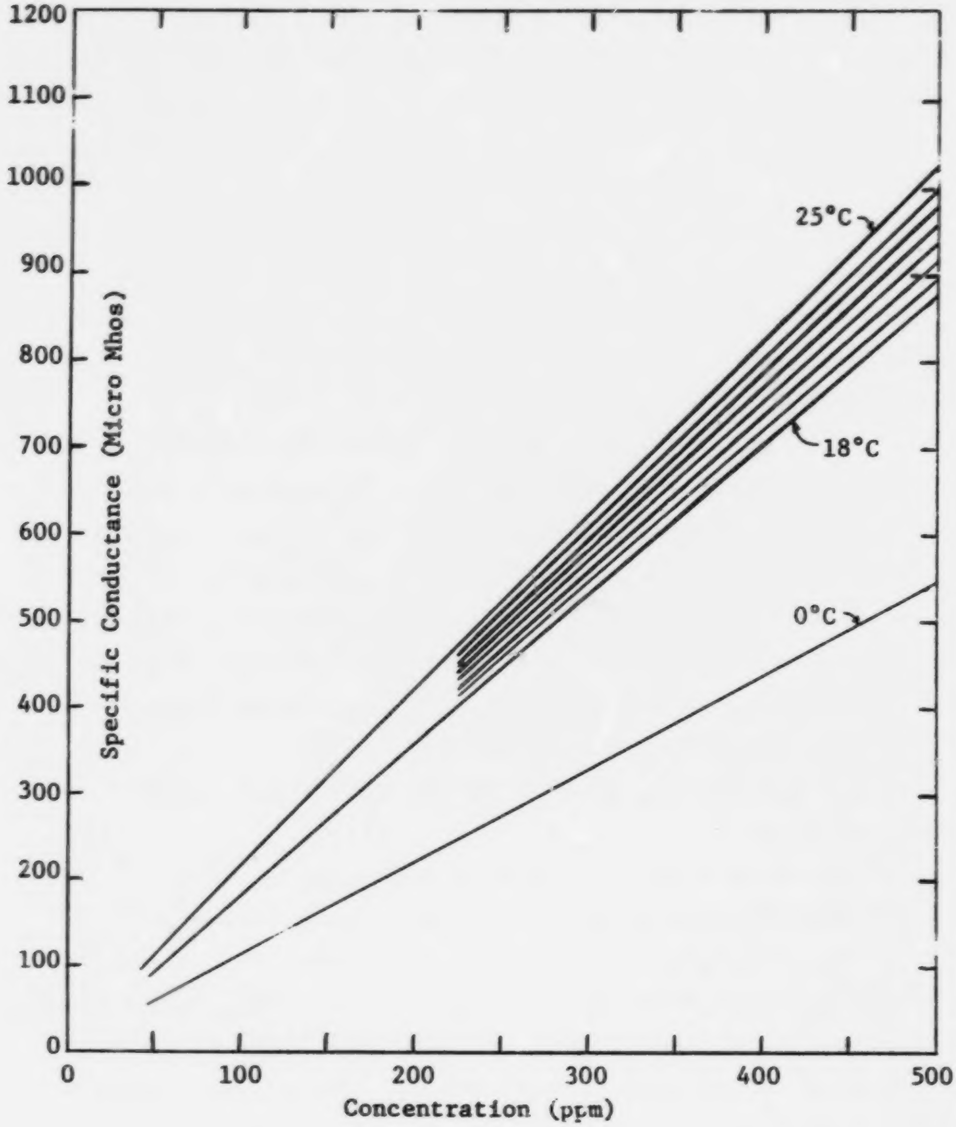


Figure 5-5: Specific Conductance of Sodium Chloride

Samples from inside the media can be taken only when the concentration is steady. The method used for sampling is described in Section 5.2.3. A conductivity probe was used for measurement of time varying concentrations.

A conductivity probe consists of two conducting electrodes some distance apart, connected to some type of electrical bridge by which the resistance of the probe can be determined. The electrodes are either placed directly in the porous media (see e.g. [5]), or mounted on a stem. The resistance of the probe is a function of the conductance of the fluid between its electrodes. The resistance also depends on the geometry of the electrical field, which is determined by the geometry of electrodes, their spacing, and the geometry of the porous medium in which the probe is located.

A conductivity probe measures the concentration over some finite volume in the porous medium. This can be considered the concentration at a point, if the size of the electrical field of the probe is small compared with some characteristic length of the flow field. It should be realized, however, that the reading is an average over some volume. When the concentration distribution has a strong curvature, the averaging will result in a flatter measured curve.

A new probe was constructed for the present study. It was designed to

(a) have a small electrical field, and

(b) be movable inside the medium along a line.

Fig. 5-6 shows the details of the probe. It was made of a 1/4" circular Phenolic resin rod. A hole was drilled perpendicular to the rod's length, and a ϕ0.100" Platinum wire was placed in it and cemented into place. The rod was turned 90° and a 1/32" slot was machined through the rod and the wire. The Platinum wire was thus cut in two, the cut faces of the two pieces serving as electrodes. The other end of each piece was connected by a thin wire, which was embedded in a groove along the rod, to an Amphenol connector. The ends of the machined slot were filled with Epoxy resin to leave a 1/4" long slot.

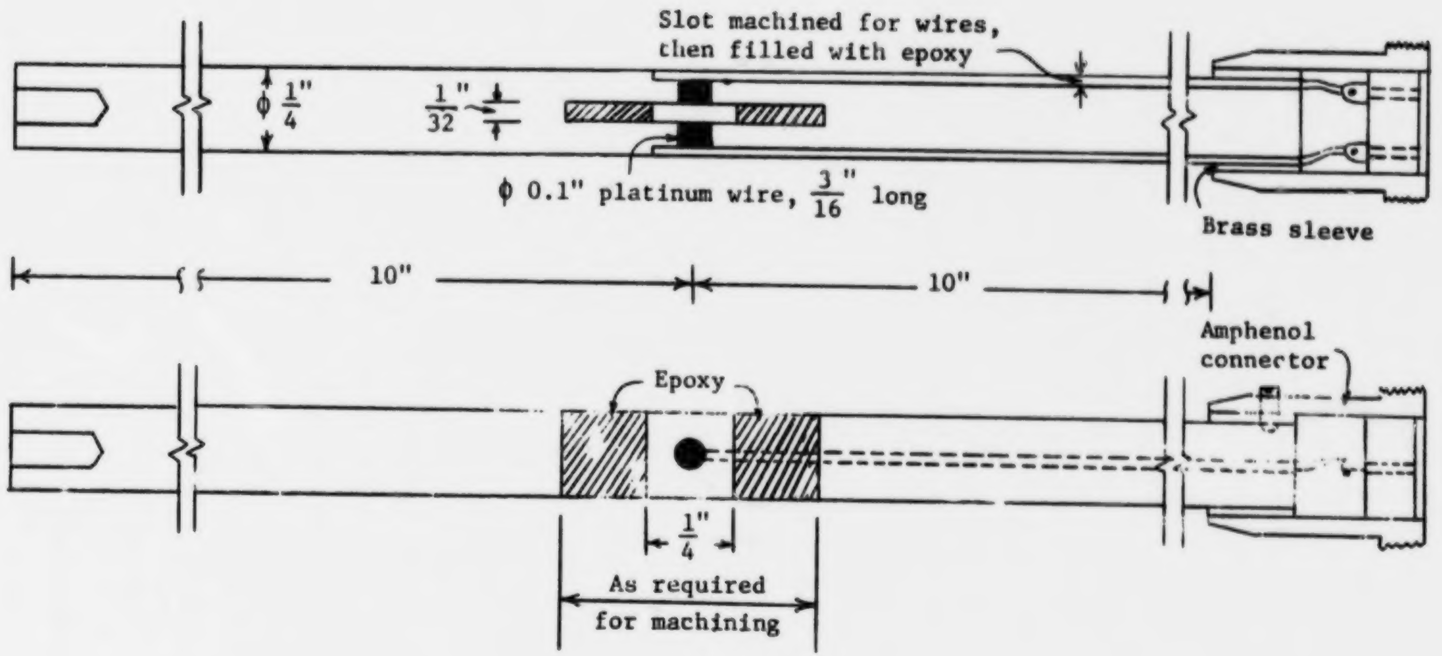

Slot machined for wires, then filled with epoxy
$\phi\ \frac{1}{4}$"
$\frac{1}{32}$"
ϕ 0.1" platinum wire, $\frac{3}{16}$" long
Brass sleeve
10"
10"
Amphenol connector
Epoxy
$\frac{1}{4}$"
As required for machining

Figure 5-6: Details of Conductivity Probe

For the low velocities the change in the flow field caused by the presence of the probe is small. The width of the slot is narrow enough not to allow sand grains to fall in, and large enough so the flow through it is not retarded relative to the flow in the surrounding media.

The outer surface of the probe is smooth so it did not disturb the medium when it was moved. The probe is sensitive to rotation, so a pointer was fixed on the stem outside the test section to indicate both angle and position.

The electrodes were coated periodically with Platinum black. This improves greatly the time response of the probe, as well as the stability of the probe. The procedure for coating is described in the Operating Manual, Type RC conductivity Bridges, Industrial Instruments, Inc.

The cell constant of a conductivity probe is defined by

$$\phi = \gamma P \tag{5-100}$$

where γ = specific conductance of the fluid, mhos/cm

P = probe resistance, ohms

ϕ = cell constant, cm^{-1}.

Combining equations (5-98) and (5-100) yields for the concentration

$$C = \frac{\phi}{\beta P} \tag{5-101}$$

ϕ = const. when the electrical field does not change (as e.g. by sand grains falling into the slot). If equation (5-99) holds, i.e. if β = const, we get for the relative concentration

$$\frac{C - C_{min}}{C_{max} - C_{min}} = \frac{(1/P) - (1/P)_{min}}{(1/P)_{max} - (1/P)_{min}} \tag{5-102}$$

The resistance of the probe was measured with a Model 350 Sanborn Recorder. The bridge configuration is shown in Fig. 5-7. For steady concentration distribution the procedure was as follows:

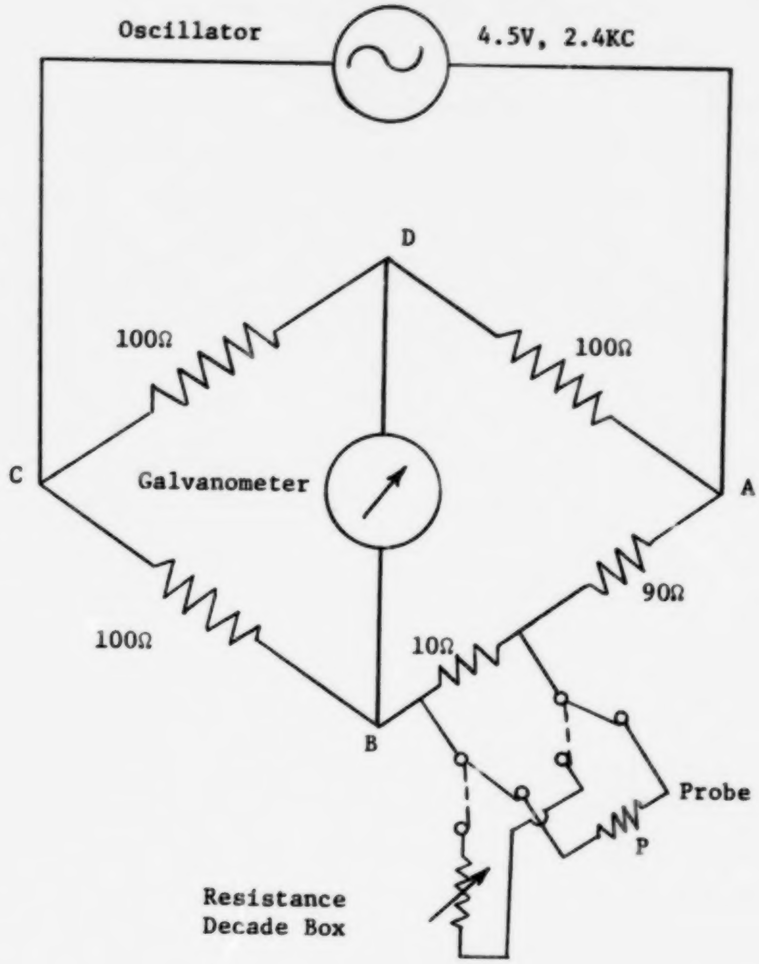

Oscillator
4.5V, 2.4KC
D
100Ω
100Ω
C
Galvanometer
A
90Ω
100Ω
10Ω
B
Probe
P
Resistance
Decade Box

Figure 5-7: Wheatstone Bridge for Sanborn Recorder

a. Balance the Sanborn with the probe in the bridge.

b. Disconnect the probe and connect in its place a resistance decade box.

c. Adjust the resistance of the decade box to rebalance the bridge. The resistance read on the box is that of the probe.

d. Move the probe to a new point and let it reach a stable resistance.

Operating the bridge always at a balanced position gives the highest sensitivity. This procedure is not suitable for the time varying concentration, so the deflection of the pen on the Sanborn chart had to be used.

The total deflection of the pen in the Sanborn Recorder is linearly related to the change of resistance between A and B.

$$\Delta R = \alpha \cdot \delta \tag{5-103}$$

where δ = total deflection = (actual pen deflection) x (attenuation)

α = coefficient depending on the Sanborn setting

ΔR = total change in resistance of leg AB.

ΔR is related to the change in probe resistance, ΔP, by

$$\Delta R = \frac{100\ \Delta P}{(10 + P_{bal})(10 + P)} \tag{5-104}$$

where P_{bal} is the probe resistance at balance.

If α is known the probe resistance for any total deflection δ is given by

$$P = \frac{10\left[\alpha\ \delta + \frac{10\ P_{bal}}{10 + P_{bal}}\right]}{10 - \left[\alpha\ \delta + \frac{10\ P_{bal}}{10 + P_{bal}}\right]} \tag{5-105}$$

α is measured as follows: after the Sanborn has been balanced for the run the probe is replaced in the bridge by the resistance decade box. The resistance of the box is set to a few resistances covering the range of probe resistance during the run, and the corresponding total deflection is measured. ΔR is calculated from equation (5-104) and plotted vs. δ. A straight line is passed through the points using least square fitting and its slope is α. This value is then used to convert total deflections during the run into probe resistances.

It is important to keep in mind the assumptions β = const and ϕ = const, implicit in equation (5-103), when using it. For example, a probe used to measure the concentration of flowing water should be balanced in flowing water. Stagnant fluid between the electrodes is heated by the current passing through it, and its conductance changes.

5.2.2 Longitudinal Dispersion

The experiments for the verification of the results of Section 5.1.1 were conducted in circular column made out of lucite (Fig. 5-8). The column had an inner diameter of 8-1/4" and a total length of 36". The flow was from top to bottom, and is governed by two constant head tanks and a regulating valve. The constant head tanks were kept at a fixed elevation, and the rate of flow was adjusted by the valve, located on the pipe between the exit from the column and the downstream constant head tank. A quick operating valve was located on the same pipe. The discharge was measured in a calibrated volumetric tank.

Six piezometer taps, 6" apart, were drilled in the wall of the column and connected through two manifolds to a manometer with an accuracy of 0.001'. Three locations for inserting conductivity probes through the column walls were also provided.

The entrance section to the column consisted of a sheet metal cone which acted as a transition from a 2" pipe to the test section. This assured a flat velocity profile in the media.

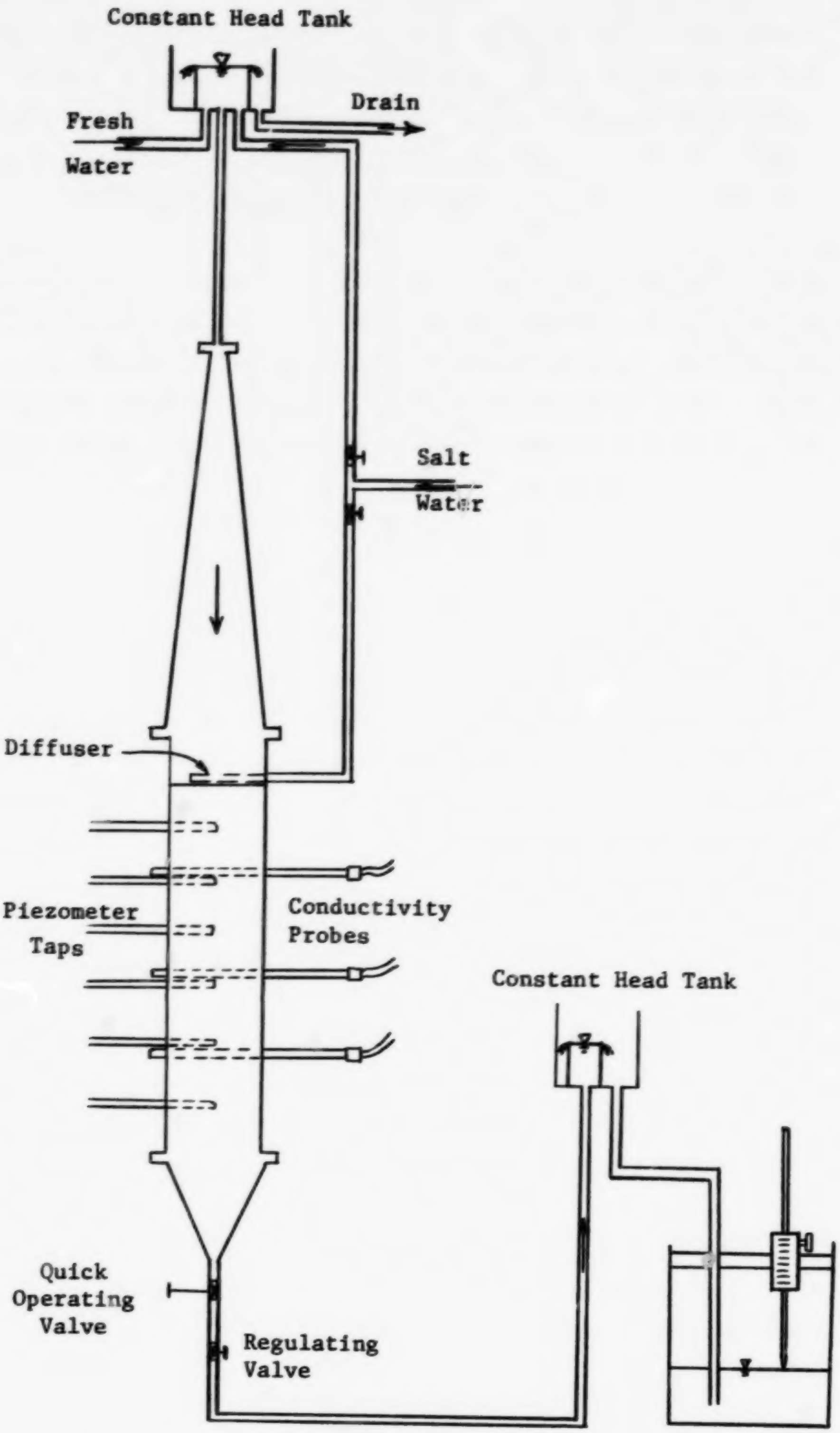

Constant Head Tank
Drain
Fresh Water
Salt Water
Diffuser
Piezometer Taps
Conductivity Probes
Constant Head Tank
Quick Operating Valve
Regulating Valve

Figure 5-8: Longitudinal Dispersion Equipment

The porous media used were different fractions of granular Silica sand. The grain size of each sand was very closely log-normally distributed. Data for the sands used is given in Table 5-1.

Table 5-1: Sands used in Longitudinal Dispersion Experiments

Sand No.	d_{50} (mm)	$UC = \frac{d_{60}}{d_{10}}$	$\sigma_g = \frac{\log d_{84.1}}{\log d_{50}}$
0	0.80	1.34	1.188
2	1.73	1.43	1.259
3	2.55	1.46	1.249
4	3.48	1.17	1.086

The sand was placed in the column in small batches, and each was compacted in place using an ϕ8-1/8" circular plate of lucite on a long handle. As it was desired to have a layered system, with sharp interfaces between the layers, vibration or rodding could not be used as compacting techniques. The porosity of each layer in situ was calculated from the volume of the layer and the weight of sand put into it. The whole formation was supported from below by a metal screen, and confined from above by another screen which was fixed to the column walls.

The column was filled with deaerated water slowly from below to allow all the air in the voids to escape. Deaerated water was allowed to flow through the column for a few days to assure complete saturation of the sand.

Before each run the medium was thoroughly flushed with fresh deaerated water. During this time the regulating valve was set to the desired flow for the next run. The probes were connected to the Sanborn Recorder and it was balanced, while fresh water was flowing in the column. The water in the entrance section was drained down to the upper surface of the sand ($x_1 = 0$). The quick operating valve on the exit pipe was then closed. The whole entrance section from the top of the media to the upstream constant head tank was filled with a salt solution in deaerated water. This water was put in at the top of the media through a diffuser at a very low rate. This assured a sharp interface between fresh and salt water at the top of the sand column.

The salt solution was 0.2% NaCl (by weight). This concentration corresponds to a difference in density of 0.1% between fresh and salt water, which can be neglected as a driving force in the displacement process. To check this a few runs were duplicated with fresh water displacing salt water. These runs gave results identical with the previous ones, and it was concluded that the difference in density had a negligible effect.

The run was started by opening the quick operating valve. While being opened the valve activated a micro-switch which produced a mark for $t = 0$ on the Sanborn chart. For the low velocities used the flow reached steady state almost instantaneously after opening the valve. Salt water was fed into the upstream constant head tank, and the discharge was measured during the run.

As the dispersed salinity front passes by the probes, the resistance of the probes changes, and this is recorded on the moving Sanborn chart and then converted into concentration (see Section 5.2.1).

5.2.3 Lateral Dispersion

Lateral dispersion tests were conducted in a Lucite box which contained the media in a section 120" long, 3" wide and 6" deep (Fig. 5-9). The porous medium rested directly against the bottom and sides of the box, whereas from above it was compressed by a strip of sponge rubber, held down by the top plate. The compressed sponge expanded to fill any gaps caused by the settling of the media with time, and thus prevented any flow short-circuiting along the top of the medium.

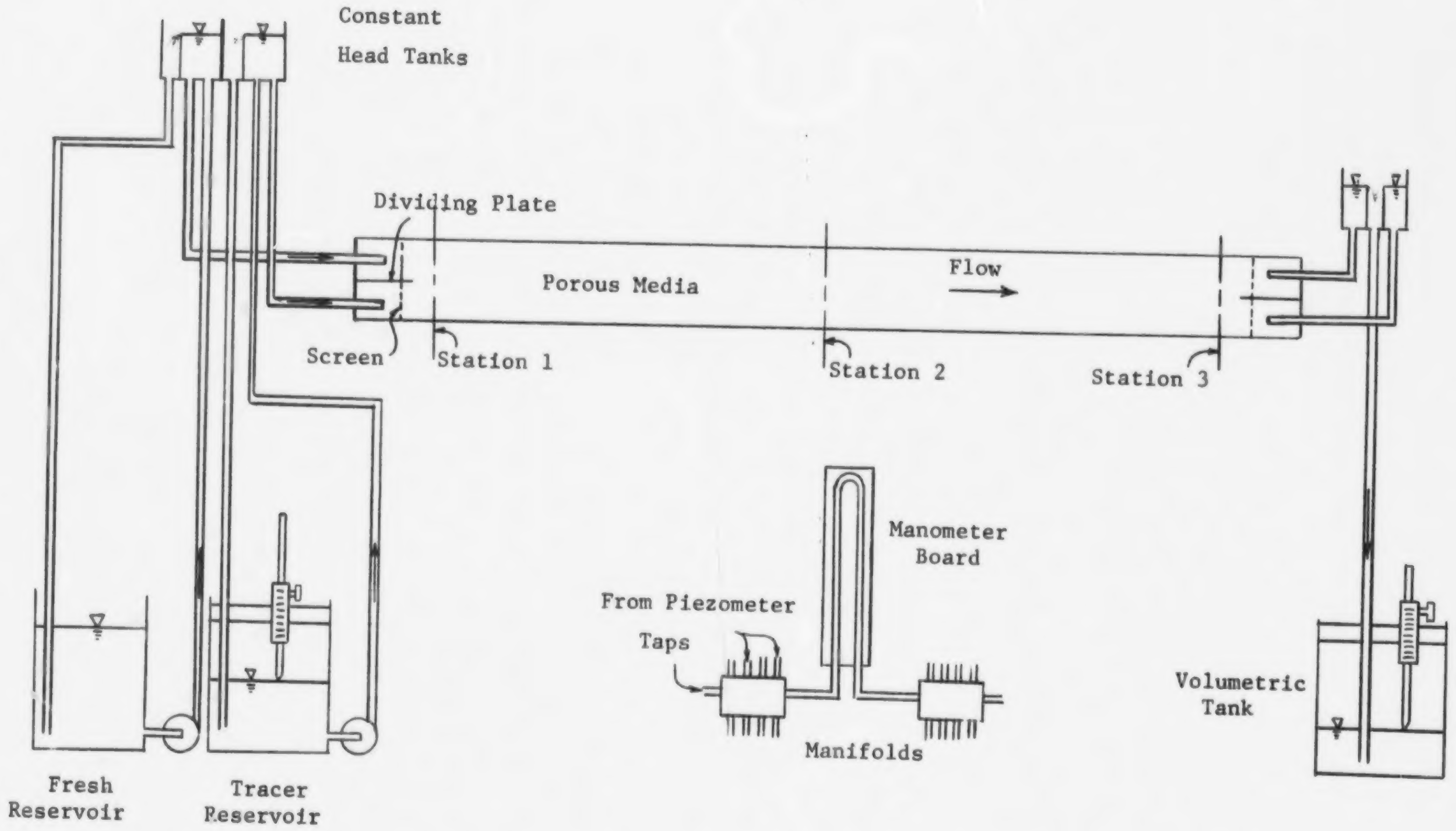

Constant
Head Tanks
Dividing Plate
Porous Media
Flow
Screen
Station 1
Station 2
Station 3
Manometer
Board
From Piezometer
Taps
Manifolds
Volumetric
Tank
Fresh
Reservoir
Tracer
Reservoir

Figure 5-9: Lateral Dispersion Equipment

The medium was confined between two screens at the ends of the box. Beyond these screens the entrance and exit sections for the flow were each divided by a horizontal Brass plate into two separate chambers. The plate extended through the screen 1-1/2" into the media. Salt water was introduced on one side of the plate and fresh water on the other (see Fig. 5-9).

The end of the plate on the inflow side was taken as the origin of the coordinate axes. This is the point at which the salt and fresh water first come in contact. The x-axis is horizontal at mid-height of the media and the y-axis vertically upwards.

Three stations were located along the box at $x_1 = 1.75$ cm, $x_2 = 149$ cm and $x_3 = 296$ cm, and called stations 1, 2 and 3 respectively. At each station there were provisions for inserting a conductivity probe in a vertical position. The probes used, of the slot type (see Section 5.2.1), could be moved vertically to get a reading at any y. At each station there were three piezometer taps in the side wall, at y = 0" y = + 1-1/2" and y = - 1-1/2". Each of the nine taps had two tubes coming out of it, each connected to one of two manifolds. Each manifold was connected to one side of a differential manometer with an accuracy of 0.001' of water. Thus the head from each tap could be compared with any other. The same tap could be connected to both sides of the manometer to check the null position, and to make sure there was no air in the tubes. Head drop along the flow was measured separately for each half of the length.

Fresh and salt water batches were prepared using deaerated water for both. Two constant head tanks were built with two separate chambers in each. (Fig. 5-9). The overflow weirs of both chambers are at the same elevation, and the overflow outlet was separate. These tanks were used one for the inflow into the box and the other for the outflow. At the inflow, fresh water was fed into the box on one side of the dividing plate through one chamber of the constant head tank, and salt water on the other side of the dividing plate through the other chamber. The overflow from each chamber went back into its reservoir. The salt water reservoir was calibrated volumetrically and provided with a point gauge. Thus the total amount of salt water used during a period of time could be measured.

At the downstream end the flow from each half of the medium was fed into one chamber of the constant head tank, thus maintaining the whole outflow section at a constant head. The overflow from both chambers was put into a volumetric tank, and the total discharge could thus be determined.

Separate measurement of the salt water discharge Q_s, and the total discharge Q_t gave the ratio of fresh water $Q_f = Q_t - Q_s$, to Q_s. Q_s and Q_f were adjusted at the beginning of each run to give a horizontal flow. The desired ratio Q_f/Q_s for each run was calculated from the permeabilities of the upper and lower half of the medium in the box (for a homogeneous medium $Q_s = Q_f$).

Measurement of Concentration Distribution

In addition to the probe located at each of the stations and read with Sanborn Recorder (see Section 5.2.1), a set of 15 sampling tubes was installed at each station (see Fig. 5-10). The samplers were made from a thin stainless steel tube (0.095" O.D.). They were located 1 cm apart on a vertical line with the middle one at $y = 0$. The tubes had a short bend and their tip was squeezed to form a very thin horizontal opening. Each sampling tube was connected through a thin Tygon tube to a sampling head. The head had fifteen stainless steel outlets, each corresponding to one sampler. All outlets were at the same elevation, and the whole head could be moved vertically on a traversing mechanism. Fifteen bottles were arranged on a rack under the sampling head to collect the samples. The samples were taken at a very slow flow rate, and after the tubes had been flushed for a long time.

Media

Two sands were used for experiments in homogeneous media. Both sands had an approximately log-normal distribution of grain size. Data is given in the following table.

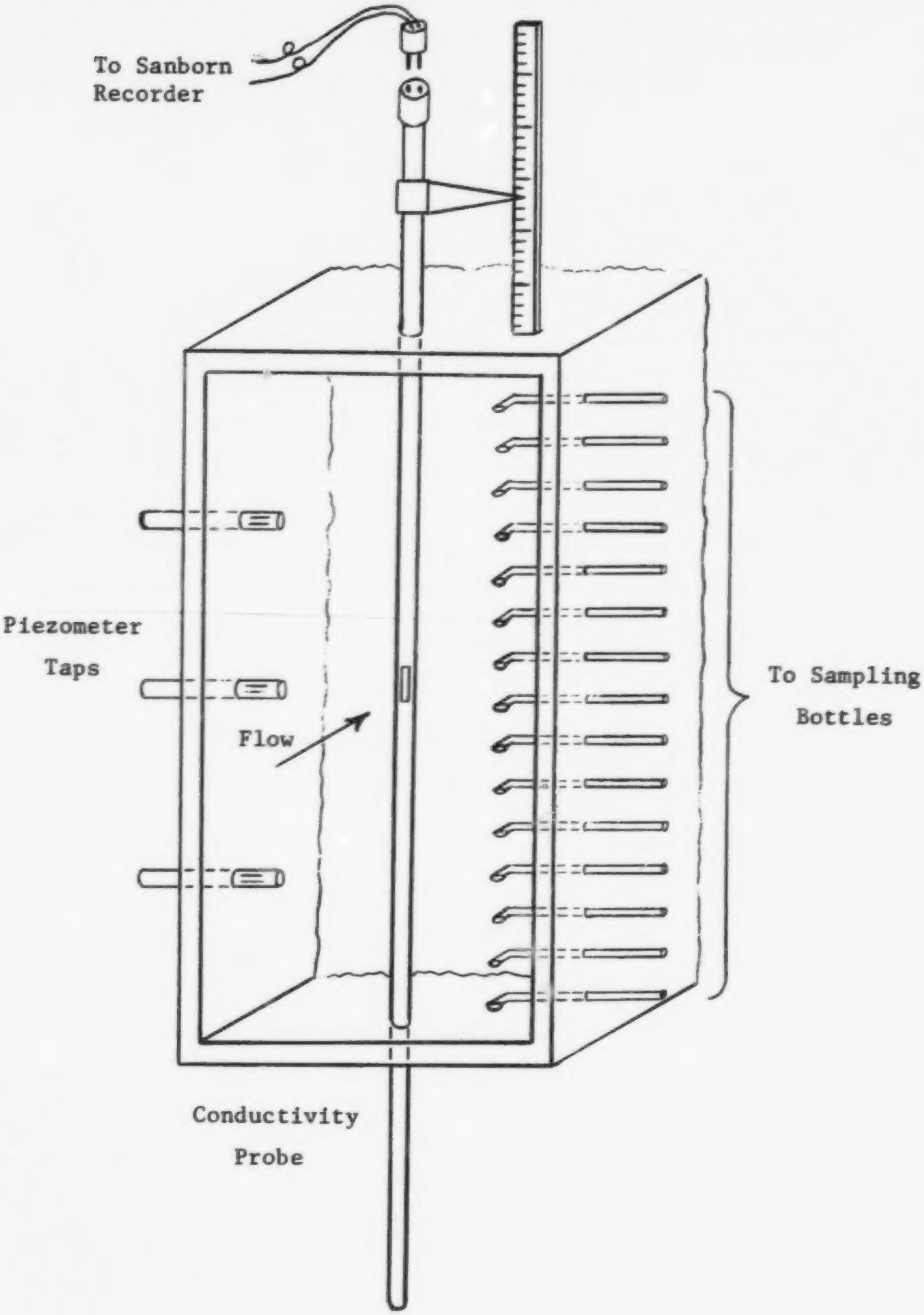

To Sanborn Recorder
Piezometer Taps
To Sampling Bottles
Flow
Conductivity Probe

Figure 5-10: Details of a Measuring Station in Lateral Dispersion Box

Table 5-2: Media used in Lateral Dispersion Experiments

Material	d_{50} (mm)	$UC = \frac{d_{60}}{d_{10}}$	$\sigma_g = \frac{\log d_{84.1}}{\log d_{50}}$
Sand # 1	1.09	1.54	1.27
Sand # 2	1.73	1.43	1.26

The layered medium was made of a layer of sand 2, extending from the bottom of the box to $y = b_1 = 2.0$ cm, and a layer of sand 1 from $y = 2.0$ cm to the top of the box.

5.3 Presentation and Discussion of Results

Results of the experiments descirbed in the previous chapters are compared with the theory and with results of the numerical scheme. In this chapter concentrations are treated as experimental results, with the understanding that they have been obtained either from samples or with a conductivity probe.

5.3.1 Longitudinal Dispersion in Homogeneous Media

In calculating the breakthrough curve for longitudinal dispersion in a layered medium one has to use the coefficients of longitudinal dispersion of each layer (see Section 5.1.1). The coefficients are obtained from experimental correlation of the dispersion coefficient with the Reynolds number. These experiments are conducted in homogeneous media. A brief summary of the experimental procedure, and some results are presented next.

Equation (5-5) is used as the expression for longitudinal dispersion in homogeneous-isotropic porous media. With the definitions $\xi = u_1 t/\ell_1$ and $\eta = D_{L_1}/u_1\ell_1$ the equation (5-5) may be written

$$\frac{C(\eta,\xi)}{C_0} = \frac{1}{2}\,\mathrm{erfc}\left(\frac{1-\xi}{2\sqrt{\eta\xi}}\right) \tag{5-106}$$

For each value of ξ the concentration C is measured. Then one can find the value of $(1 - \xi)/2\sqrt{\eta\xi}$ from equation (5-106) using a table of the error function. When $(1 - \xi)/2\sqrt{\eta\xi}$ is plotted vs. $(1 - \xi)/2\sqrt{\xi}$ on arithmetic paper the slope of the straight line (a best fit through the experimental points) is $\sqrt{\eta}$. D_{L_1} can then be calculated using the definition of η. Results are correlated using equations (2-4), (2-5) or (2-6). The values of the coefficients in these equations vary between different investigators. It is believed that for longitudinal dispersion experiments, where one has to measure a transient concentration, these differences stem largely from differences in the technique used for measuring concentrations. Much of the experimental work reported in the literature was done with concentrations being measured as an average over the whole outflow cross-section. Optical methods are common (a dye detected by a light source and photo-cell arrangement). This method yields usually values of D_L which are larger than those measured with a conductivity probe inside the medium (see discussion of ref. [2]).

The correlation used in this work are those given by Harleman, Mehlhorn and Rumer [29]. Their method for measuring concentration was essentially the same as that used in this study.

The equation used was

$$\frac{D_L}{\nu} = 0.9\left(\frac{u\, d_{50}}{\nu}\right)^{1.2} = 0.9\, \mathbb{R}_{d_{50}}^{1.2} \qquad (5\text{-}107)$$

5.3.2 Longitudinal Dispersion in a Layered Medium

Two series of runs were conducted to verify the results presented in Section 5.1.1.

Runs 41-45: alternating layers of sands # 0 and # 3 (see Table 5-1), each 1.25" thick.

Runs 51-55: layer 1, 25.1 cm of sand # 1
layer 2, 30.5 cm of sand # 2
layer 3, 30.5 cm of sand # 4

In this series the conductivity probes were located at the end of layers 2 and 3.

The seepage velocity for each layer was calculated, using the measured discharge Q and the porosity of the layer θ_i, from

$$u_i = \frac{Q}{\theta_i A} \tag{5-108}$$

(with $A = 339.5\ \text{cm}^2$). Then D_{L_i} was calculated from equation (5-107). The theoretical breakthrough curve is calculated from equation (5-23).

For runs 41-45 the individual layers of each sand were "lumped" into one equivalent layer for the calculation of the breakthrough curve. For each probe the lengths of all the layers of each sand were added up and the total length was used. The order in which these two layers were considered is immaterial, as was pointed out at the end of Section 5.1.1.

Figure 5-11 gives the comparison of theoretical, numerical and experimental results for Run 45, at Station 3. The data used are

layer no.	sand no.	ℓ (cm)	u (cm/sec)	D_L (cm^2/sec)
1	0	41.6	0.154	0.0115
2	3	41.3	0.154	0.0465

A calculation was carried out with the order of the layers reversed (i.e. sand no. 3 is layer no. 1), and it gave identical results.

Results for Run 52 at Station 2 and 3 are presented in Figures 5-12 and 5-13 respectively.

The data for Run 52 are:

layer no.	sand no.	ℓ (cm)	u (cm/sec)	D_L (cm^2/sec)
1	0	25.1	0.127	0.0097
2	2	30.5	0.123	0.0214
3	4	30.5	0.121	0.0528

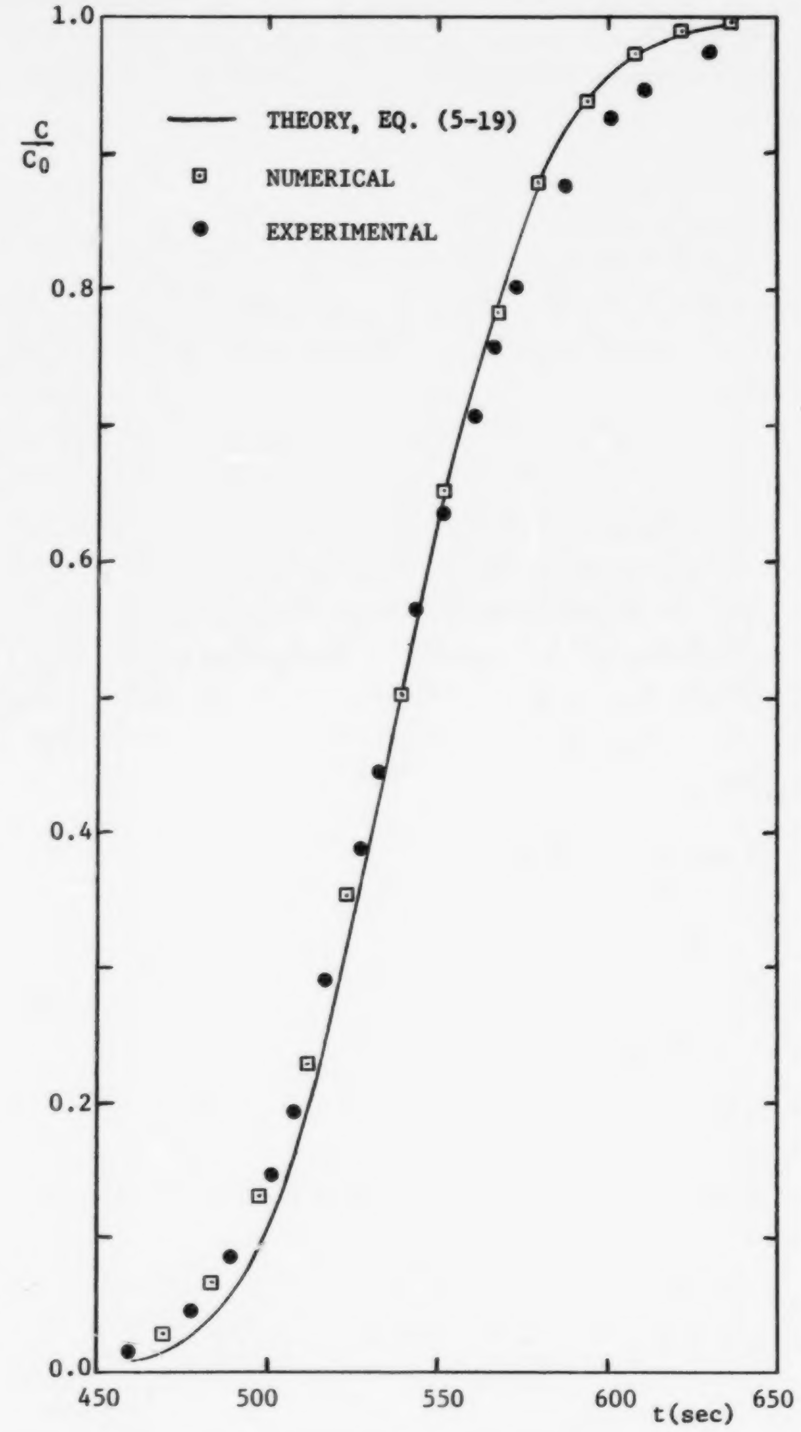


Figure 5-11: Theoretical, Numerical and Experimental Results for Run 45, Station 3

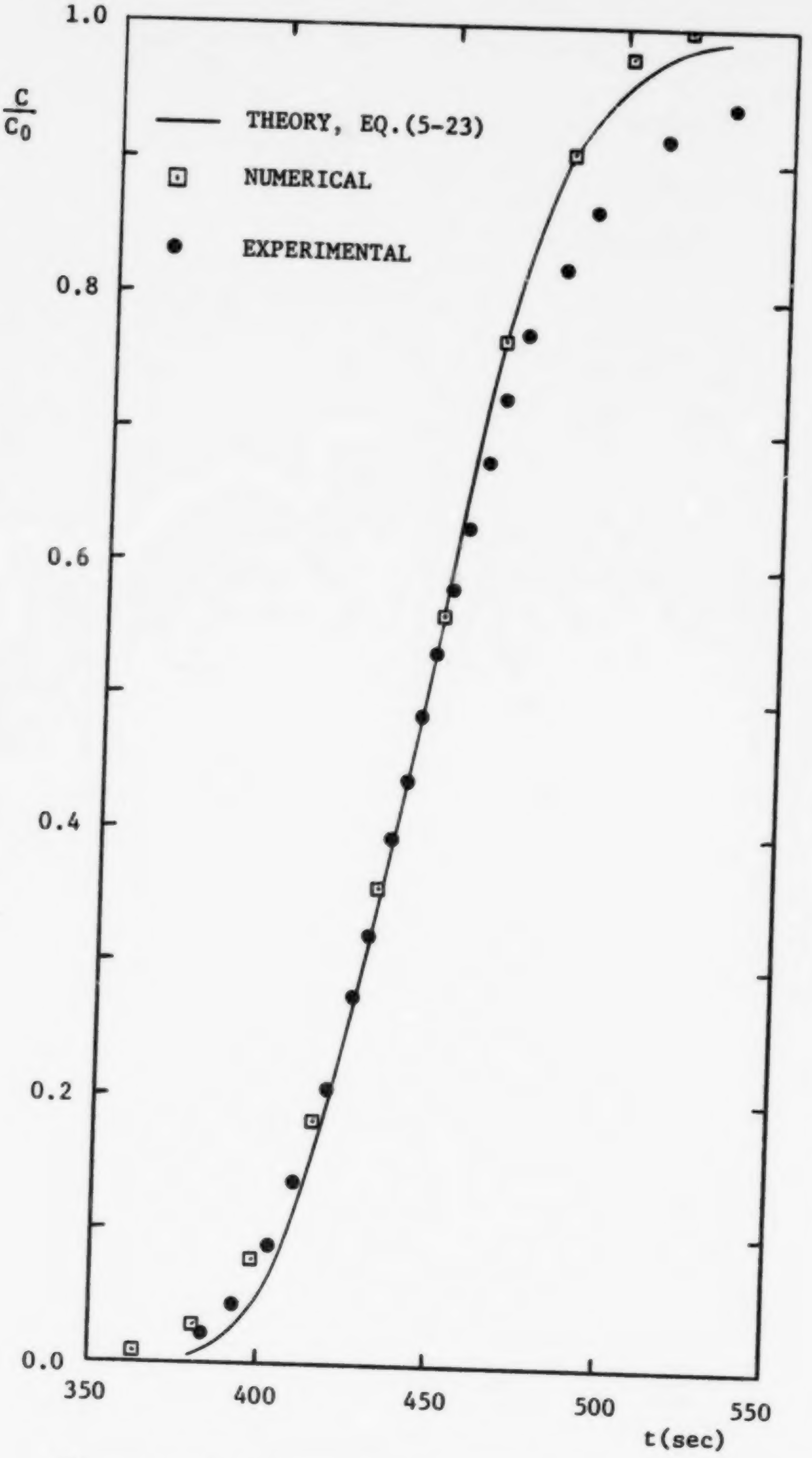


Figure 5-12: Theoretical, Numerical and Experimental Results for Run 52, Station 2

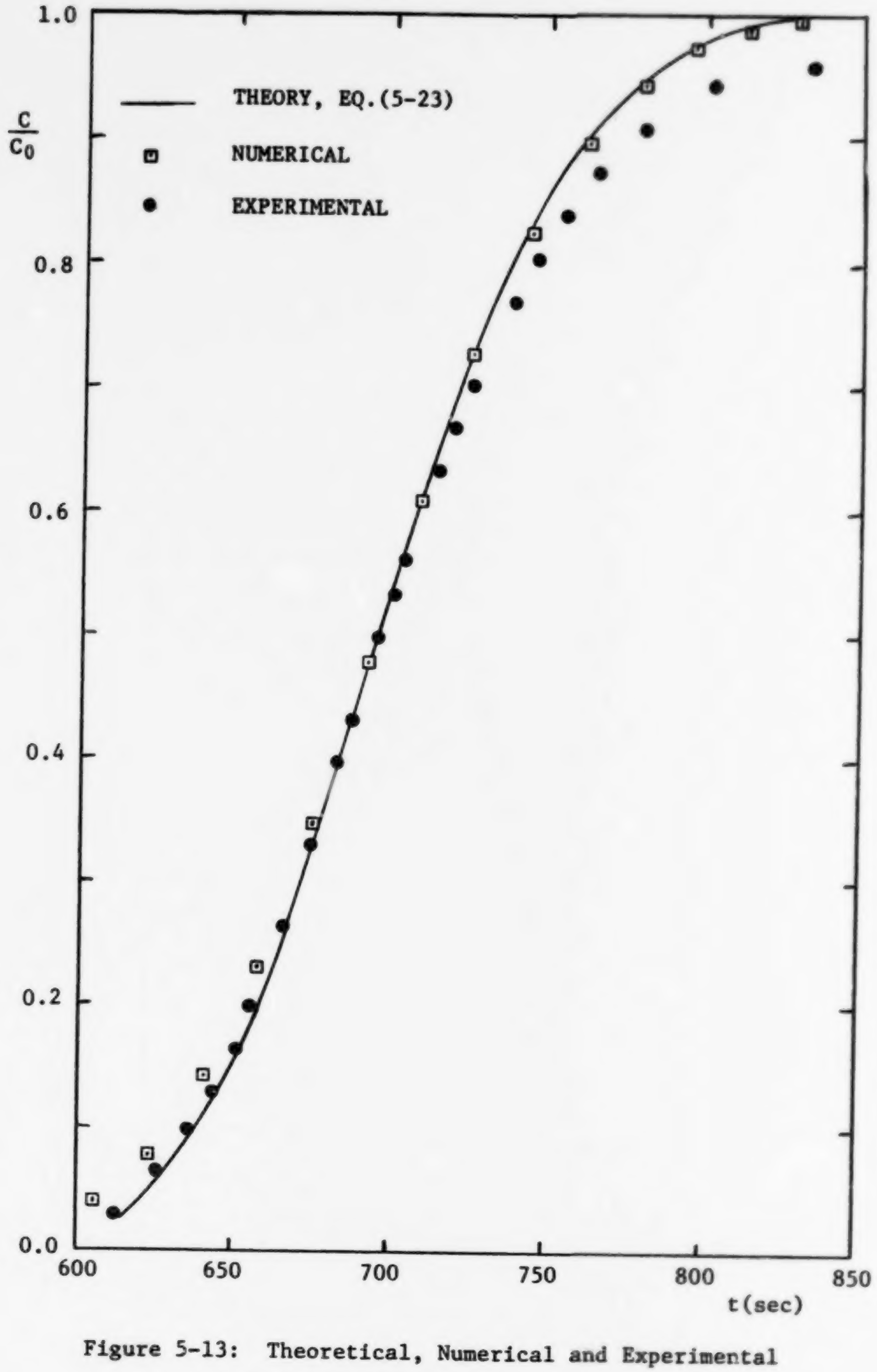


Figure 5-13: Theoretical, Numerical and Experimental Results for Run 52, Station 3

Station 2 and 3 are the end of layers 2 and 3, respectively.

The other runs in each series covered a wide range of seepage velocities. The results presented here are typical. In all runs the experimental values of C/C_0 were lower than the theoretical and numerical results for the late part of the curve. This was attributed to mixing into dead pore spaces, which traps part of the tracer material, and is equivalent to an effective adsorption. This effect was neglected in the differential equation, which does not include an adsorption term.

The theoretical curves were calculated with values of D_L given by equation (5-107), and the results indicate that this equation is a valid relation.

Another method of analysis of the experimental results was tried. One may consider any medium in which longitudinal dispersion takes place as a homogeneous medium, in the absence of information about the individual layers. This is a "black-box" approach in which one seeks the parameters of the system which characterize its behaviour with respect to the mixing process occurring in it.

The experimental results are treated as a breakthrough curve of an equivalent medium, which is homogeneous and isotropic. The length of the equivalent medium, ℓ_{eq}, is the total length of the layered formation (i.e. the sum of the lengths of the individual layers). The equivalent seepage velocity, u_{eq}, is computed from the time of arrival of the point $C/C_0 = 0.50$ at the exit section, denoted by t_{50}. Then $u_{eq} = \ell_{eq}/t_{50}$. Using ℓ_{eq} and u_{eq} in equation (5-5) the equivalent dispersion coefficient of the formation, $D_{L_{eq}}$, is computed by the method outlined in Section 5.3.1. This value is then used in equation (5-5) to compute the "equivalent" breakthrough curve. This curve is a best fit of equation (5-5) to the experimental results. The degree of agreement of the equivalent curve with the experimental results merely indicates to what degree the shape of the experimental curve may be described by equation (5-5).

Figures 5-14 and 5-15 give the equivalent curves for Station 3 in Runs 45 and 52, respectively. It is seen that for Run 45,

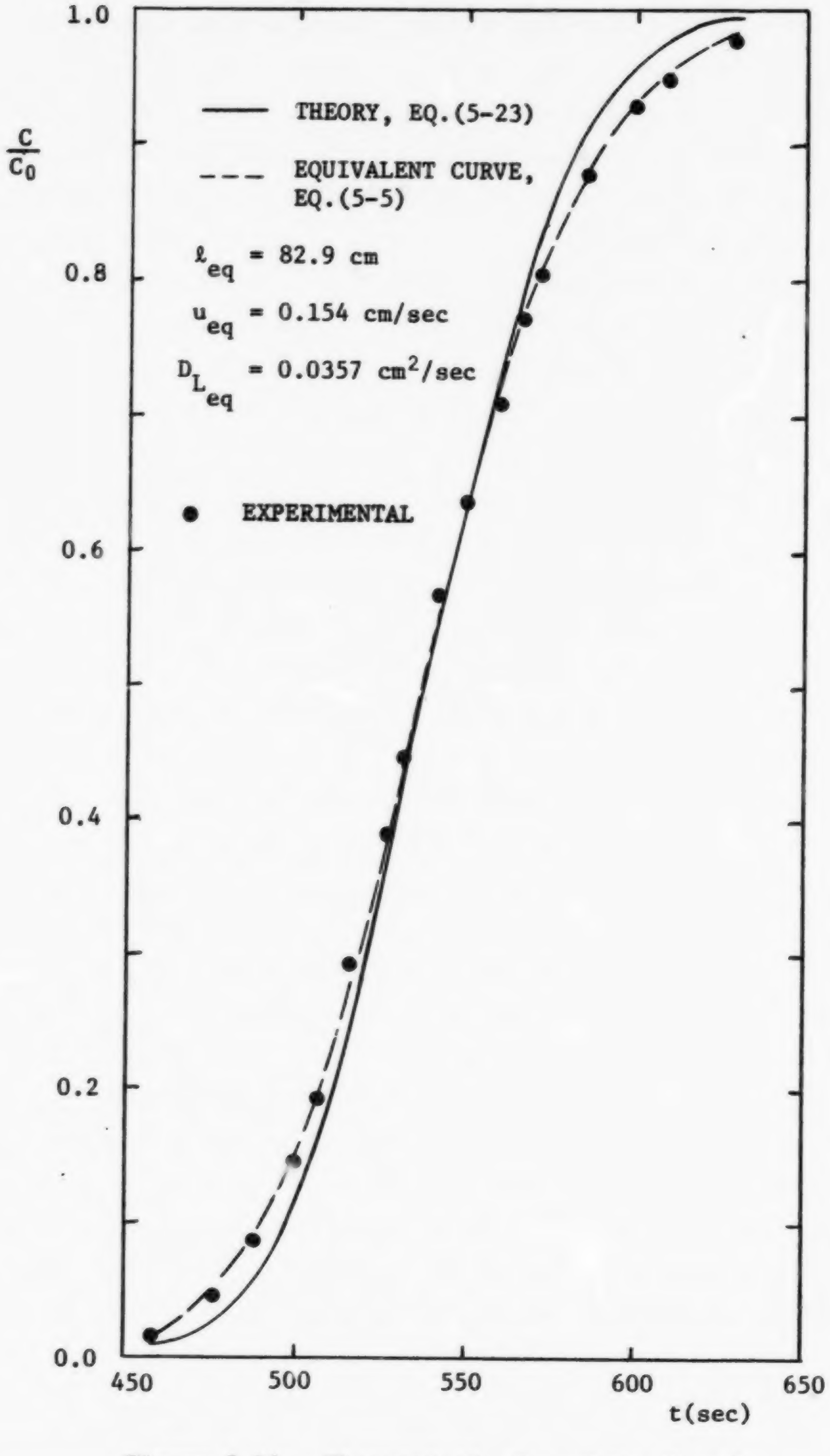


Figure 5-14: Theoretical, Experimental and "Equivalent Medium" Results for Run 45, Station 3

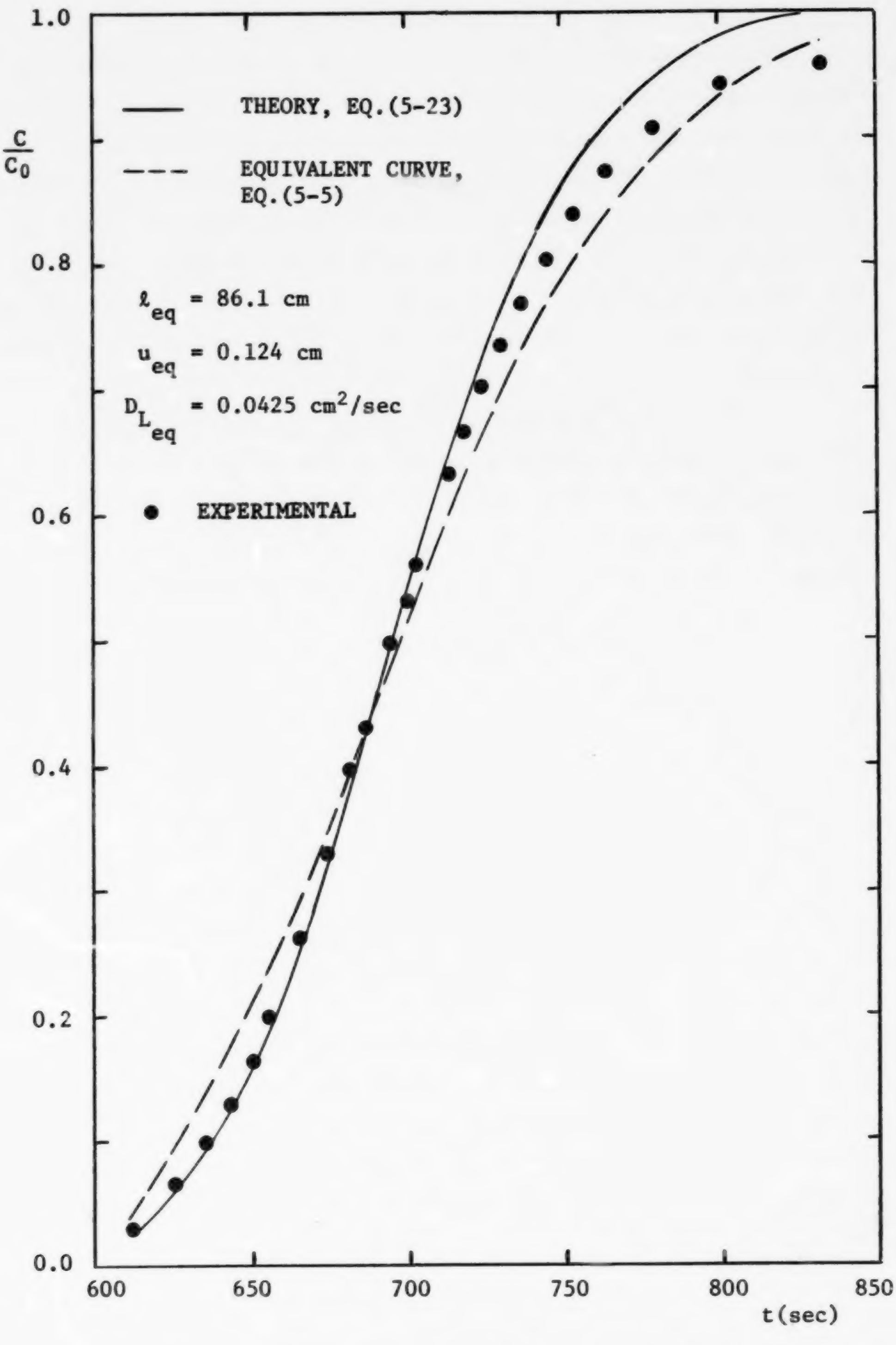


Figure 5-15: Theoretical, Experimental and "Equivalent Medium" Results for Run 52, Station 3

in which there are only two layers, the agreement is better than for Run 52, in which there are three layers.

Other investigators have used the fact that the experimental breakthrough curve can be described very well by equation (5-5) to infer that the medium in which they were conducting the experiments was indeed homogeneous. This is not necessarily the case, as demonstrated by the above results. Small inhomogeneities in the medium, caused by segregation of fractions during placing in the test column or by uneven compaction, will show up as variations in the value of the computed dispersion coefficient while the shape of the curve can still be expressed by equation (5-5).

As for all experimental runs the seepage velocity did not vary much from one layer to the next it was decided to check the agreement of the numerical scheme with the theory for an artificial run, in which there are two layers with very different seepage velocities. The data for this run, designated Run LL-1, are

$\ell_1 = 4.65$ cm $\qquad u_1 = 0.1$ cm/sec $\qquad D_{L_1} = 0.01$ cm^2/sec

$\ell_2 = 5.70$ cm $\qquad u_2 = 0.05$ cm/sec $\qquad D_{L_2} = 0.005$ cm^2/sec

Results are presented in Figure 5-16 for two points in the second medium, $x_2 = 4.665$ cm and $x_2 = \ell_2 = 5.70$ cm. As was the case for longitudinal dispersion in homogeneous media (Section 4.1) the results for the end of the medium are not as good as for a point inside it. This can be improved by extending the medium beyond its physical end, for purposes of computation, as explained in Section 4.1.

In computing the numerical results for longitudinal dispersion in a layered medium the grid was chosen so that a grid point coincided with the boundary between the layers. The values of the seepage velocity and longitudinal dispersion coefficient for this point are the average of the values in the two layers on either side of this boundary.

5.3.3 Lateral Dispersion in Homogeneous Media

In calculating the steady concentration distribution resulting from lateral dispersion in layered media one has to use the coeffi-

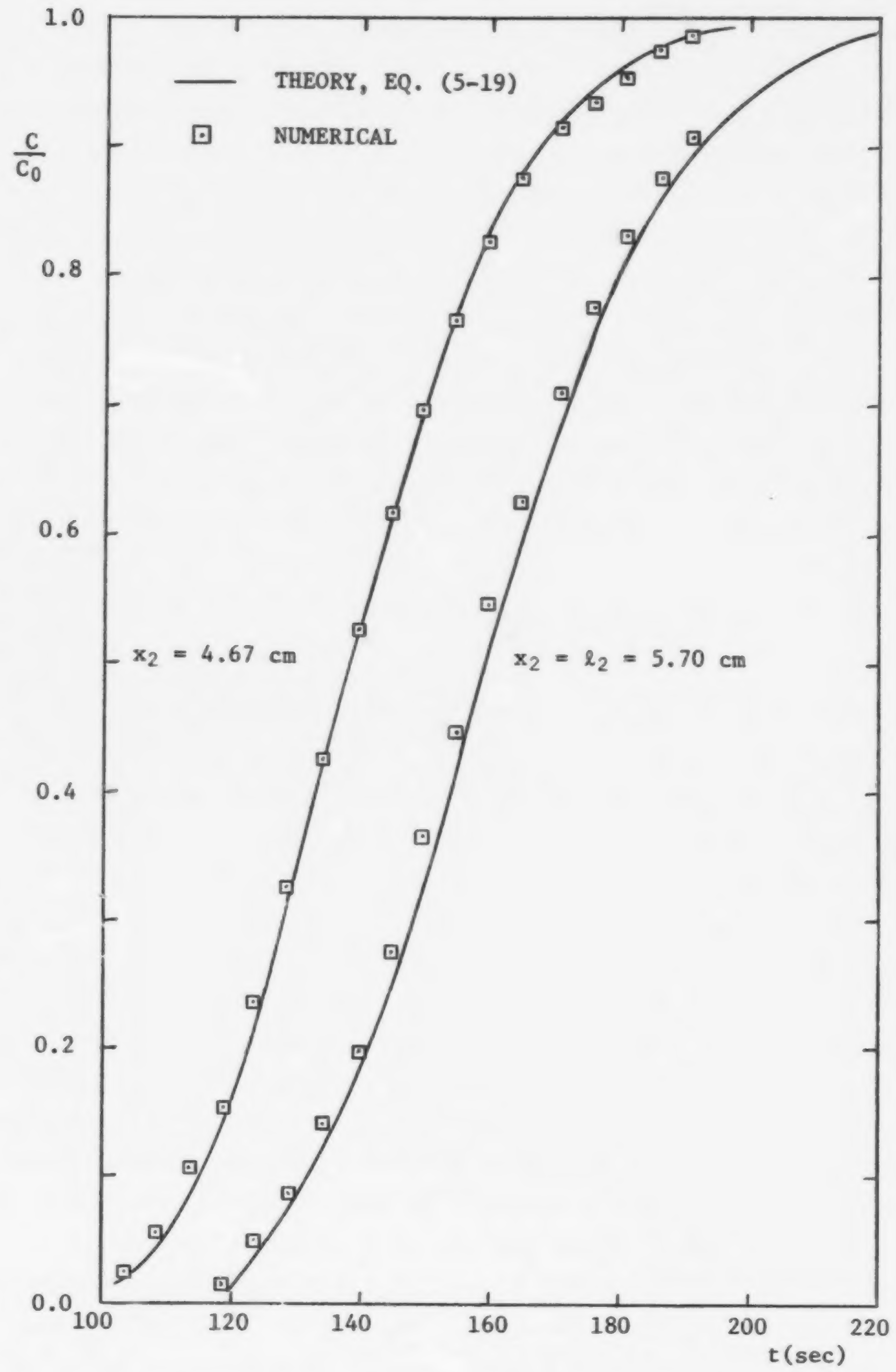


Figure 5-16: Theoretical and Numerical Results for Run LL-1

cients of lateral dispersion of each layer. (See Section 5.1.2) These values are obtained from experimental correlations of the type given in equations (2-4) to (2-6). There is no agreement among different investigators as to the values of the coefficients in these correlations. Values of D_T calculated from expressions given by different investigators may vary by as much as a factor of 10. For this reason it was decided to conduct lateral dispersion experiments in two different homogeneous sands, and then use the same sands for the layered medium.

The lateral dispersion coefficient for a homogeneous medium is calculated from measured lateral concentration distributions at a few stations along the direction of flow. The seepage velocity is calculated from the measured discharge and the medium porosity. For any x and y equation (5-73) can be written

$$\operatorname{erf}\left(\frac{y}{2\sqrt{D_T x/u}}\right) = 1 - 2\,\frac{C(x,y)}{C_0} \qquad (5\text{-}109)$$

With the measured C(x,y) one can find the argument of the error function from tables. When $y/2\sqrt{D_T x/u}$ is plotted on arithmetic paper vs. the corresponding value of $y/2\sqrt{x/u}$, and a straight line is fitted through the points, its slope is $\sqrt{D_T}$. The experimental points for both stations 2 and 3 were plotted on one plot, and the best line was fitted through all points. The value of D_T is very sensitive to changes in the slope of the line. The line fitting was done by eye, rather than by a least square method, because sometimes there were isolated points which clearly deviated from the general trend and those were dropped.

The calculated values of D_T/ν are correlated with $\mathbb{R}_{d_{50}} = u\, d_{50}/\nu$ and with $\mathbb{R}_{\sqrt{k}} = u\sqrt{k}/\nu$ in Figures 5-17 and 5-18 respectively. These correlations were used to compute the lateral dispersion coefficient of each layer in the experiments with layered media.

The samplers described in Section 5.2.2 were installed after the completion of the experiments with sand no. 1 and before the experiments with sand no. 2 and with layered media. It was found that the sampling technique gave much better results than the

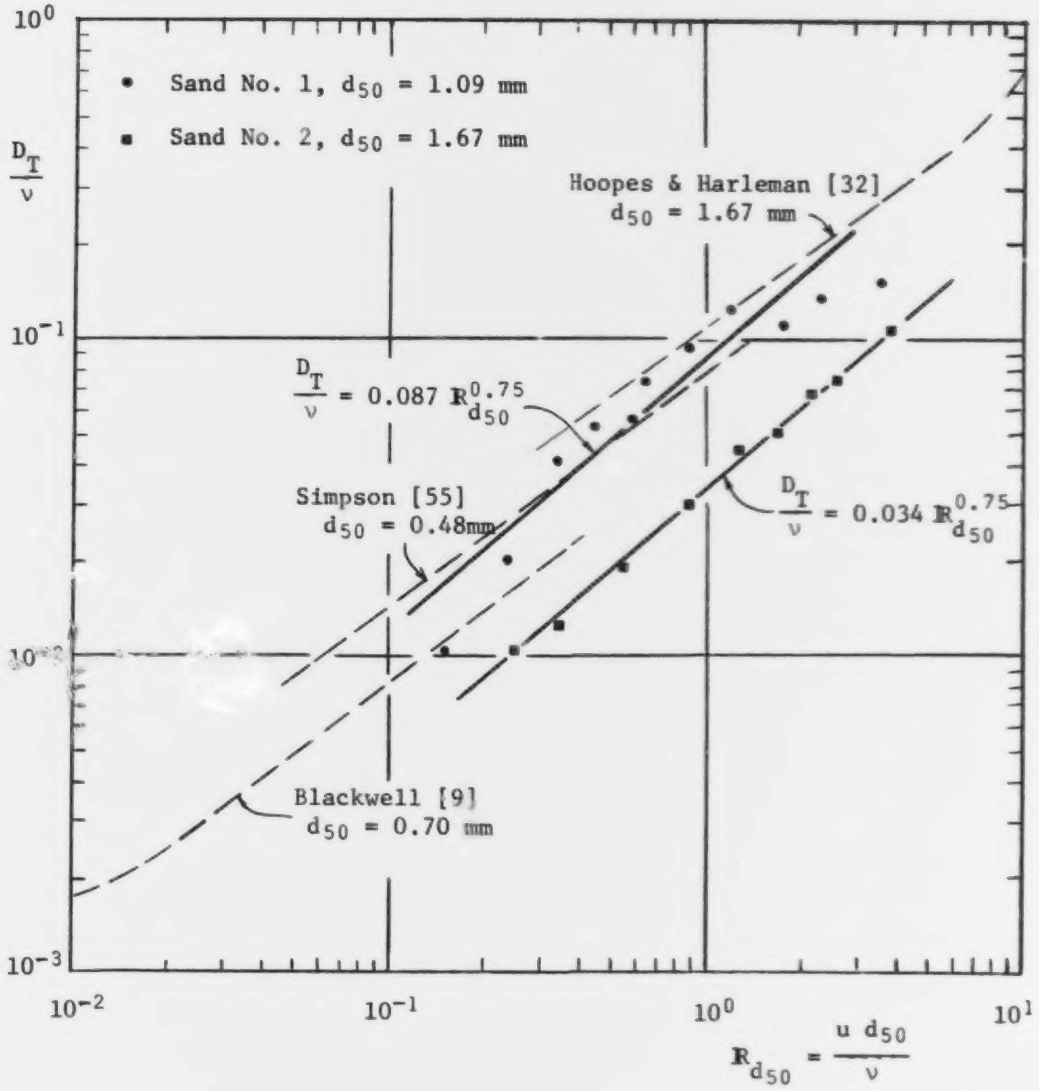


Figure 5-17: Correlation of D_T/ν with $\mathbb{R}_{d_{50}}$

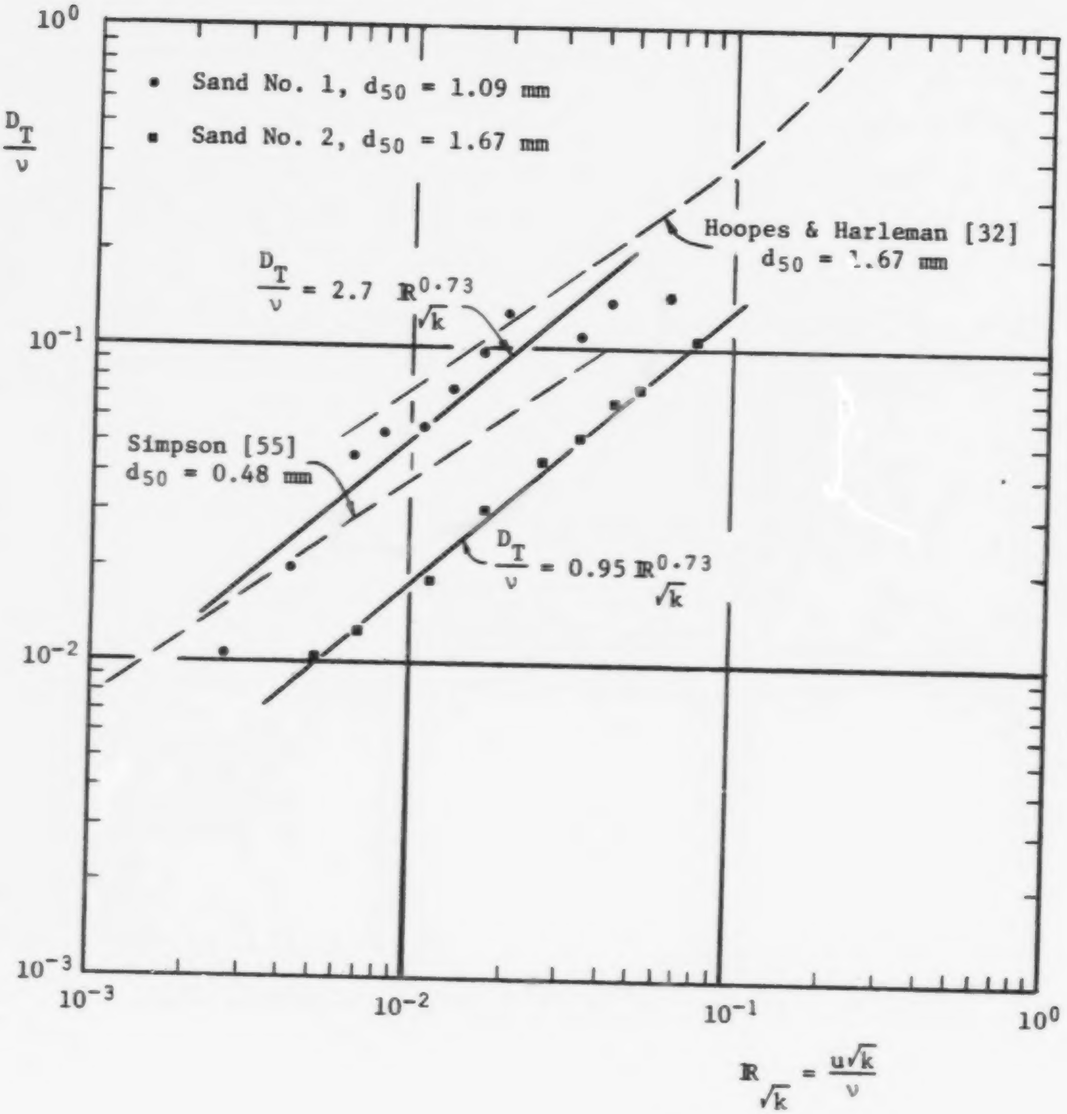


Figure 5-18: Correlation of $\frac{D_T}{\nu}$ with $\mathbb{R}_{\sqrt{k}}$

conductivity probes. The readings were more repeatable, and the calculated values of D_T gave better correlation curves. This can be seen from Figures 5-17 and 5-18 in comparing the results for sands nos. 1 and 2.

It was found in a few runs that the point $C/C_0 = 0.5$ did not coincide with $y = 0$ at one or more measuring stations. This may be caused by an unequal discharge through the two halves of the box. Especially at low flows it was difficult to keep the discharges constant. Unequal discharges produce a vertical velocity component, which causes the concentration distribution to be shifted vertically. When reducing the data from these runs the point $C/C_0 = 0.50$ was taken as $y = 0$, that is, the curve was shifted back to make $C(x,0)/C_0 = 0.50$. The shift was usually only a few millimeters, but sometimes as much as 1.5 cm.

5.3.4 Lateral Dispersion in Layered Media

A series of experiments was conducted on lateral dispersion in a medium consisting of two layers, to verify the results of Section 5.1.2. The lower layer, made of sand no. 2, extended from the bottom of the box to $y = b_1 = 2$ cm. The upper layer, made of sand no. 1, extended from $y = b_1 = 2$ cm to the top of the box. The porosities of both layers were $\theta_1 = \theta_2 = 0.345$. The layers had different permeabilities, and therefore the fresh water discharge in the upper half of the box was different from the salt water discharge through the lower half. Based on permeabilities measured during the experiments with the homogeneous sands, the ratio of salt to fresh water discharges was calculated to be

$$\frac{Q_s}{Q_f} = 1.88$$

Maintaining this ratio assured a horizontal flow in both layers. The seepage velocity in each layer was calculated from the discharge through it and the porosity. The lateral dispersion coefficient for each layer was obtained from the correlations in Figure5-17. Equations (5-70) and (5-72) were used to compute the theoretical concentration distributions.

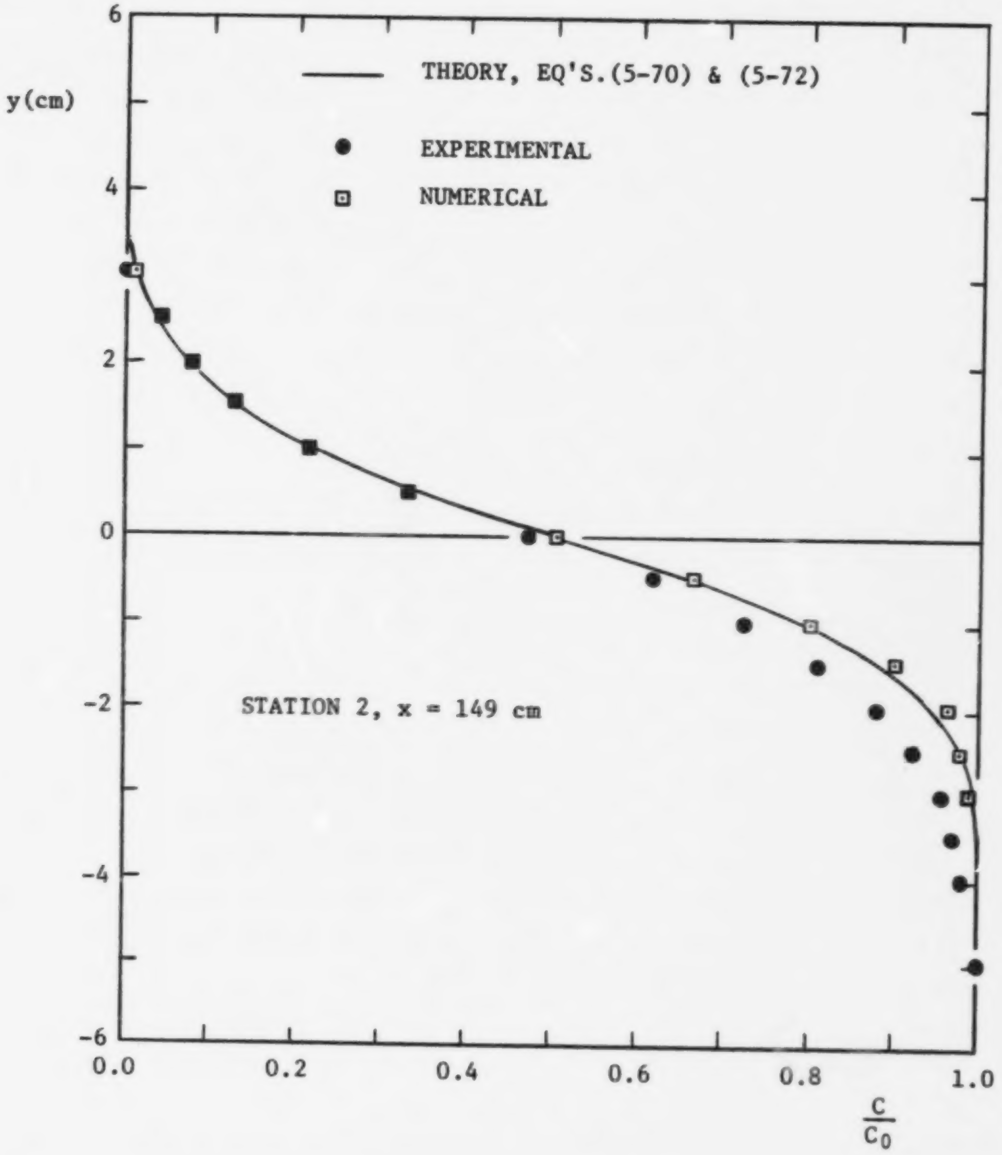


Figure 5-19: Theoretical, Numerical and Experimental Results for Run 132, Station 2

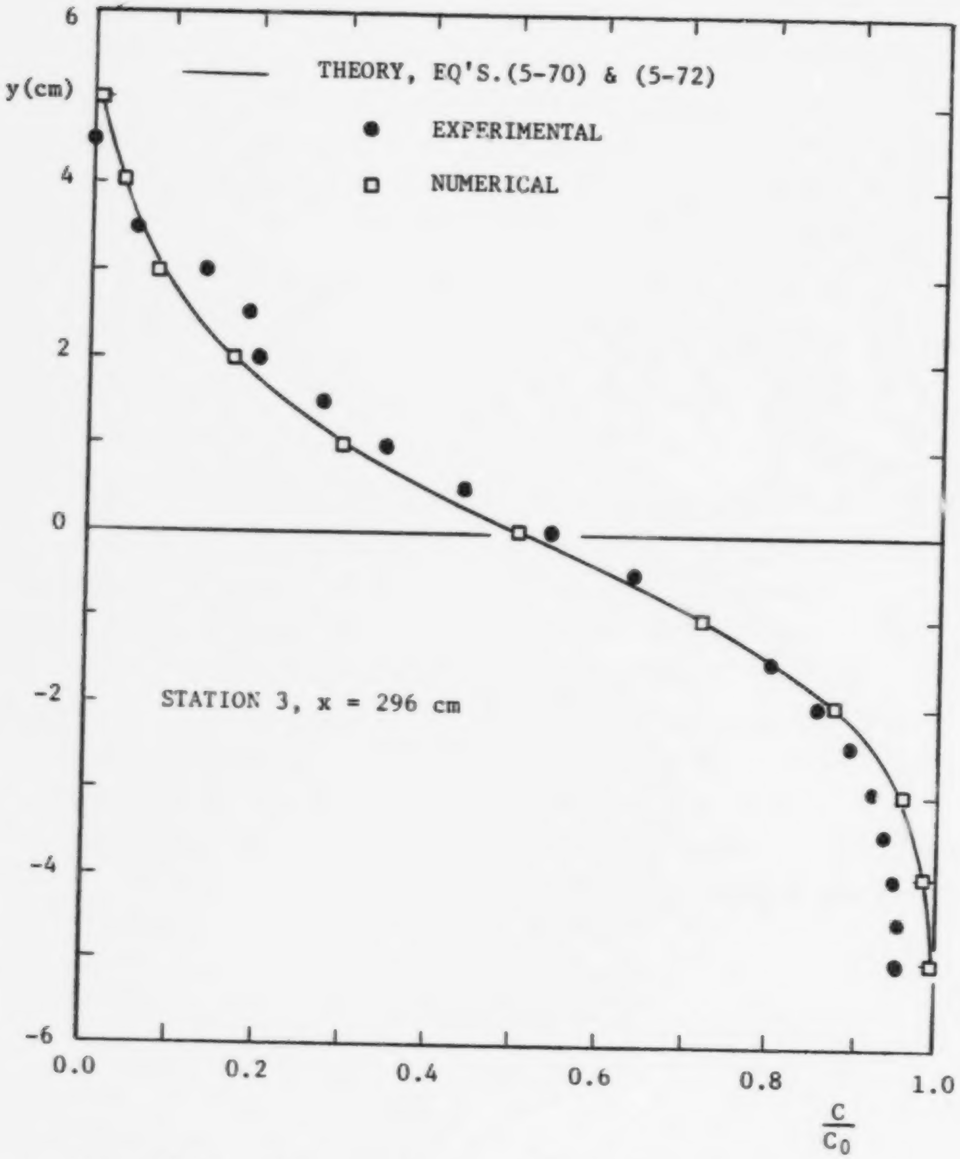


Figure 5-20: Theoretical, Experimental and Numerical Results for Run 132, Station 3

It was very difficult to maintain a constant ratio of the fresh and salt water discharges. This was especially true at low flow rates. Any deviation caused vertical velocities to be set up, and the concentration pattern to be moved vertically. For the layered media there is no way of correcting for this by a shift of the coordinates. For runs with high seepage velocities the agreement between the theoretical solution and the experimental curve was better than for low velocities.

The steady state concentration distribution at stations 2 and 3 for Run 132 were calculated from equations (5-70) and (5-72) using the following data

Layer no.	Sand no.	u cm/sec	$\mathbf{R}_{d_{50}}$	D_T cm^2/sec
1	2	0.181	3.1	9.5×10^{-4}
2	1	0.066	0.75	7×10^{-4}

The results are presented in Figures 5-19 and 5-20 for stations 2 (x = 149 cm) and 3 (x = 296 cm).

The numerical scheme, with a three equation option (the full scheme) was used to compute the steady state distribution for Run 132. As only the steady state was of interest the solution was started by putting the concentration in the whole lower half equal to 1.0, in the upper half equal to 0, and on $y = 0$ equal to 0.5. This reduced the time required for the solution. The numerical results are also given in Figures 5-18 and 5-19.

VI. SUMMARY AND CONCLUSIONS

6.1 Evaluation of the Numerical Scheme

The use of the convective dispersion equation in Φ-ψ coordinates as the basis for the numerical scheme to solve problems of dispersion in which the miscible fluids have the same density and viscosity has resulted in the following:

a. The scheme is general enough to handle any problem of dispersion in a steady flow field, with any boundary and initial conditions. It is also applicable to a special class of flow fields with unsteady flow. The solution of a particular problem requires only minor modifications of the computer programs.

b. The most efficient numerical scheme developed for the one-dimensional linear problem, the Stone and Brian scheme, can be used, with no modification, to take care of convection and dispersion in the direction of flow.

c. The dispersion at right angles to the flow is treated by an alternating direction implicit scheme, which is more efficient than either an explicit or a fully implicit scheme.

d. If dispersion at right angles to the direction of flow is neglected, an abbreviated scheme may be used, which solves for convection and longitudinal dispersion along each streamline separately. This scheme results in a substantial saving in computer time.

The scheme is applicable to dispersion in non-homogeneous media, and it is suggested that it can be used for anisotropic media as well.

The efficiency achieved by the numerical scheme makes it acceptable as a practical tool. It can be used directly to solve field problems. This may require quite large amounts of computer time as the numerical solution has to be propagated much in the same way that the physical concentration distribution changes with time. In other words, there is no way to get the numerical results for large times without carrying out the solution from the initial condition to the desired time with time increments of restricted magnitude. The numerical scheme can be used instead of a laboratory model for generating experimental results for any problem in a very short time, and at a very moderate cost. The numerical results can be used to obtain approximate analytical solutions, or to verify their validity.

The scheme was used, in this work to give results for some problems, for which no exact or approximate analytical solutions exist. These include the transient longitudinal and lateral dispersion in uni-directional flow, longitudinal dispersion in unsteady uni-directional flow, radial and source-sink flows with a pulse input.

6.2 Extension and Suggestions for Future Work

The proposed scheme is by no means the only possible one which can be written to solve the Φ-ψ equation numerically, using the Stone and Brian scheme for the convection and dispersion in the direction of the flow, and an alternating direction scheme to treat the dispersion at right angles to the streamlines. One alternative scheme, which did not prove to be very good, was mentioned. Others should be tried, as all that is involved is changing the expressions for the coefficients in the coefficient subroutines. One major modification can be suggested, however. One may consider a scheme with three implicit equations. The explicit equation in the proposed scheme does not have the structure of the Stone and Brian scheme. In certain cases this may cause the results of the second equation, namely C^{**}, to be a better solution than the final results. One may consider a third implicit equation, which is similar to the first equation, except that the Δ_ξ^2 term uses C_{n+1}^{**} instead of C_n.

Subjects, not covered in the present work, which should be investigated are:

a. Other numbers of cycles. The weighting coefficients can be computed from the expansion given by Stone and Brian.

b. Using a variable number of cycles during the solution.

For example, use 3 cycles during the early parts, when the front is sharp, and 1 cycle when the front has been somewhat dispersed.

c. Determine the effect of $D_L \Delta t/(\Delta x)^2$ on the accuracy. One may consider both $u\Delta t/\Delta x$ and $D_L \Delta t/(\Delta x)^2$ to determine the time step sequence, and use the smaller value of Δt.

d. Anisotropic media. At each point one has to compute the angle between the velocity vector and the principal axes of the dispersivity tensor to compute the dispersion coefficients. Otherwise the solution is the same.

e. Unsteady flow in cases where the streamlines and equipotentials change position with time. After each time step one has to associate the results with a fixed coordinate system, then change the location of streamlines and equipotentials and find the initial concentration of the new grid from its location in the fixed coordinate system. For this case the method of characteristics may prove to be more suitable and efficient.

f. As a special case of (e) one may consider permeability which is varying with time non-uniformly over the flow field. This may be caused by clogging, for example, in flow from a recharging well. The permeability at a point A may be considered as given by

$$k_A(T) = \int_0^T C_A(t)\ q_A(t)\ dt$$

The efficiency of the computer program can be increased for certain problems by solving the convective dispersion equation only in those parts of the flow field where the concentration is varying with time. Consider for example the one-dimensional problem in which ℓ_x is very large. During the early part of the solution one computes many zero values for concentrations at downstream points. In other words, past a certain grid point the tri-diagonal equations have all zero right hand members. During the late parts of the solution one computes many values of $C/C_0 = 1.0$ behind the moving front. This procedure is wasteful. The programs can be modified to solve a "moving portion" of space only, picking up new grid points in front and dropping old ones behind, so that only the region of space in which the concentration is still varying is solved.

This procedure is easily applicable to the one-dimensional and radial problems. The same procedure can also be used for each streamline separately, when lateral dispersion is neglected in a two-dimensional problem and the one equation scheme is used. When the full scheme is used for a two-dimensional problem one has to consider the whole field as a unit, and vary the size of the solved portion so it always includes all points at which the concentration is varying.

This procedure requires a moving boundary condition as well. For example in the one-dimensional problem one has to apply the reflection boundary condition at the first point used in front, and a fixed value boundary condition at the last point behind.

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APPENDIX A: COMPUTER PROGRAMS

The listings of two computer programs are included herein:

a. 1F1D = one-dimensional flow with one-dimensional dispersion.

b. 2F2D = two-dimensional flow with two-dimensional dispersion.

Flow charts included are:

a. Macro flow chart of MAIN - 2F2D.

b. Flow chart of the three-equation option in 2F2D. The one- and two-equation options simply eliminate parts of the full, three-equation scheme.

c. Flow chart for SUBROUTINE TDCSI used in 2F2D. This is the more general of the tri-diagonal subroutines (because it uses both C and C^* to compute the right hand side of the equations), and TDETA can be deduced from it.

No flow charts are given for the other service subroutines for 2F2D, or for the one-dimensional program 1F1D.

NOTE: 1F1D is similar to the one-equation option of 2F2D, except that a fixed value of the boundary condition on x = 0 is considered as C(1), whereas in 2F2D it is considered as C(0,J) (i.e. it is a point outside the flow field). Therefore to compare the results of 2F2D for longitudinal dispersion in uni-directional flow with the results from 1F1D, the former should have one less grid points along the streamline.

Input Data for 2F2D

(See definition of symbols in program listing)

Card # 1 FORMAT (10A6)

Title, anything on first 60 columns, will be printed at top of output.

Card # 2 FORMAT (I5, 3F10.5)

1 5
ISO

Card # 3 FORMAT (I5, 3F10.5)

1 5	6 15	16 25
IDIV	FIMIN	FIMAX

Card # 4 FORMAT (I5, 3F10.5)

1 5	6 15	16 25
JDIV	CSYMIN	CSYMAX

Note: JDIV = 0 and CSYMAX = CSYMIN for solution along a single streamline.

Card # 5 FORMAT (5F10.5)

1 10	11 20
UZERO	ELZERO

Card # 6 FORMAT (5F10.5)

1 10	11 20	21 30
ALFAL	ALFAT	DMOL

Card # 7 FORMAT (2(I3,F7.2))

1 3	4 10	11 13	14 20
KFETA	CFETA	KLETA	CLETA

Card # 8 FORMAT (2(I3,F7.2))

1 3	4 10	11 13	14 20
KFCSI	CFCSI	KLCSI	CLCSI

Card # 9 FORMAT (5F10.5)

1 10	11 20	21 30	31 40
A1	A2	A3	A4

Card # 10 FORMAT (I5, 3F10.5)

1 5	6 15	16 25	26 35
NCYC	TETA(1)	TETA(2)	TETA(3)

Card # 11 FORMAT (I5, 3F10.5)

1 5	6 15	16 25	26 35
NN	DTMIN	DTMAX	DTSTEP

Card # 12 FORMAT (I5, 3F10.5)

1 5	6 15	16 25
KIN	CSYNN	CSYNX

Card # 13 FORMAT (3I3)

1 3	4 6
IMAP	NM

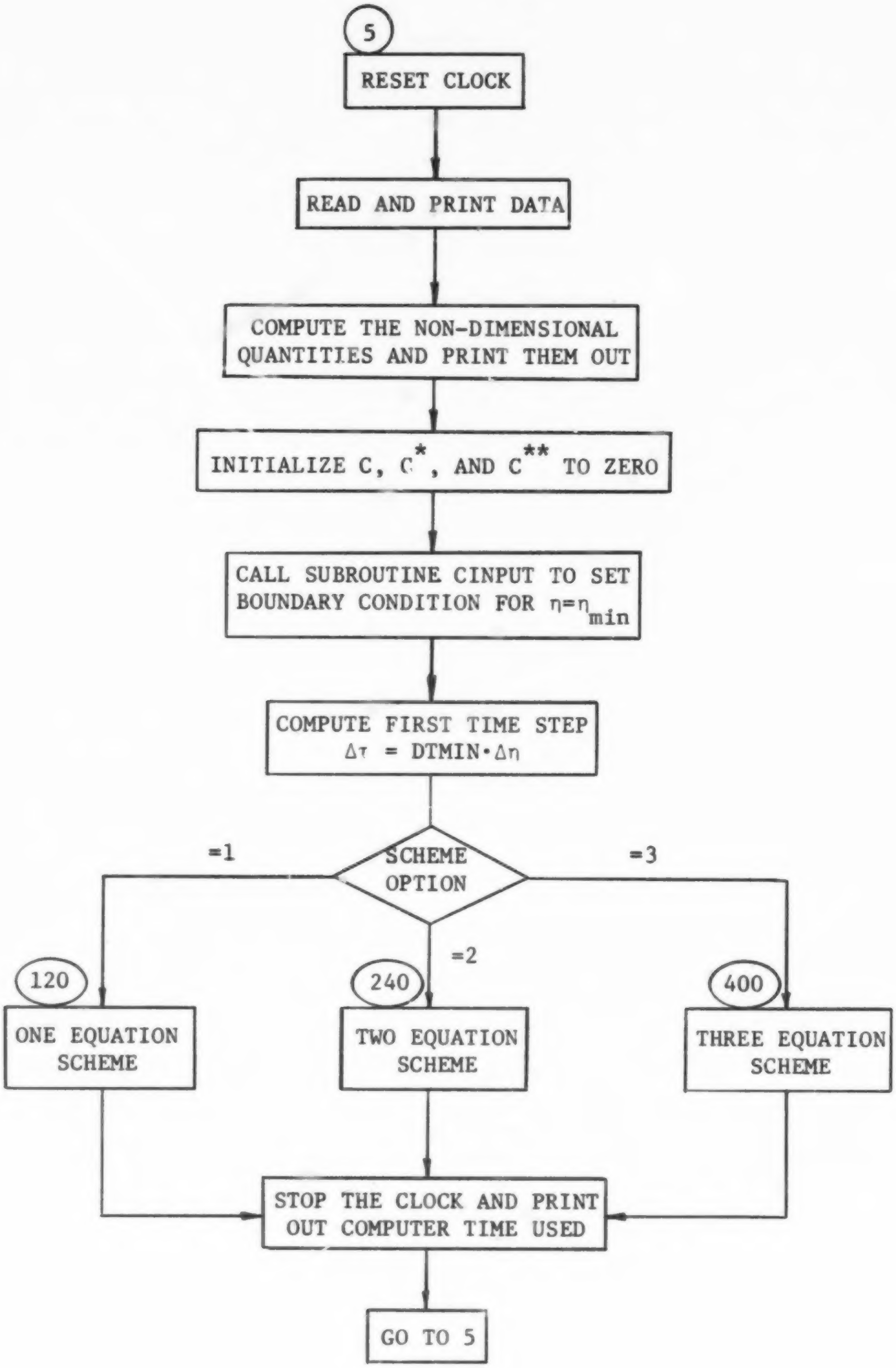
Card # 14 FORMAT (3I3)

1 3	4 6	7 9
IPRNT	ISTEP	JSTEP

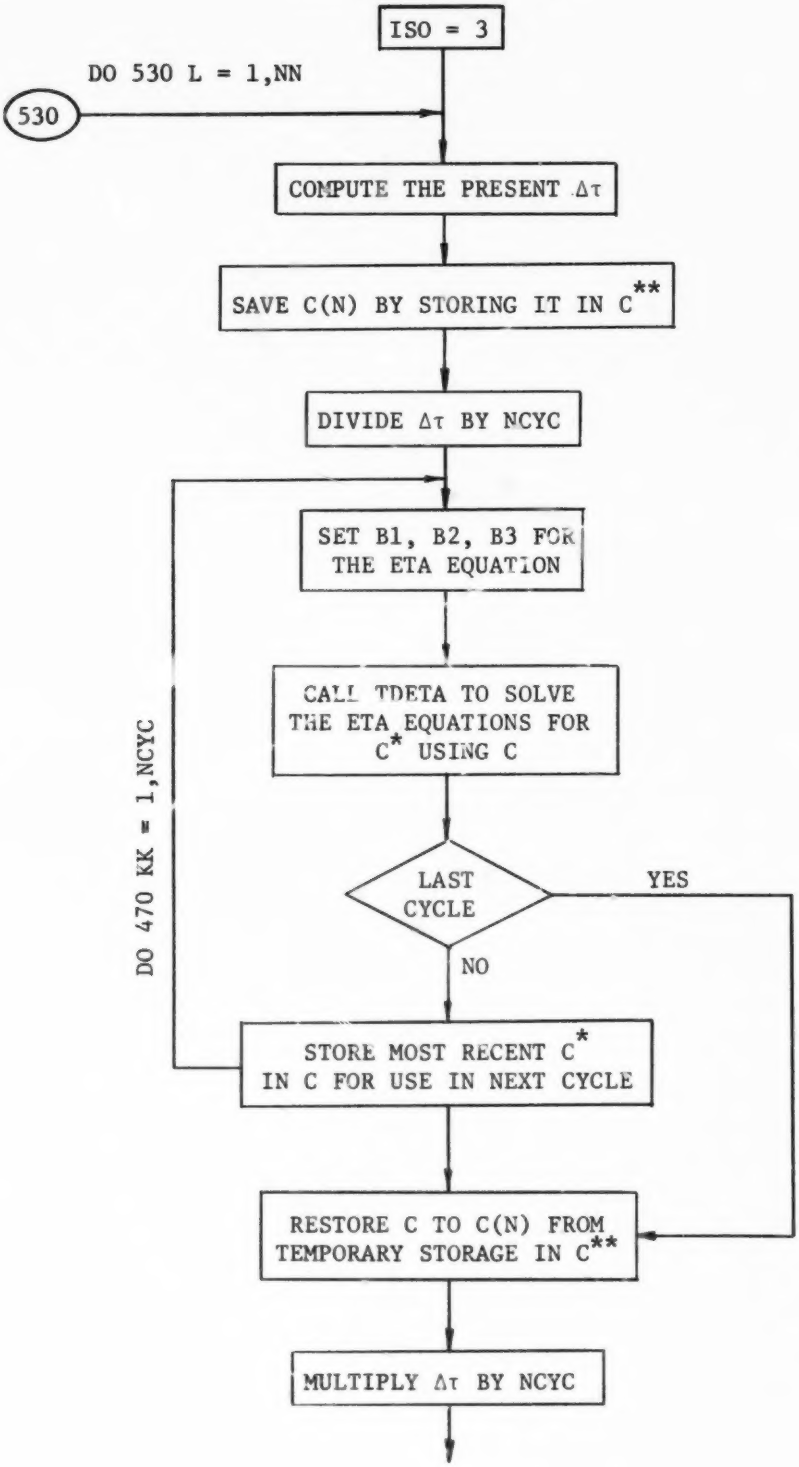
Card # 15 FORMAT (F10.5, 2I3)

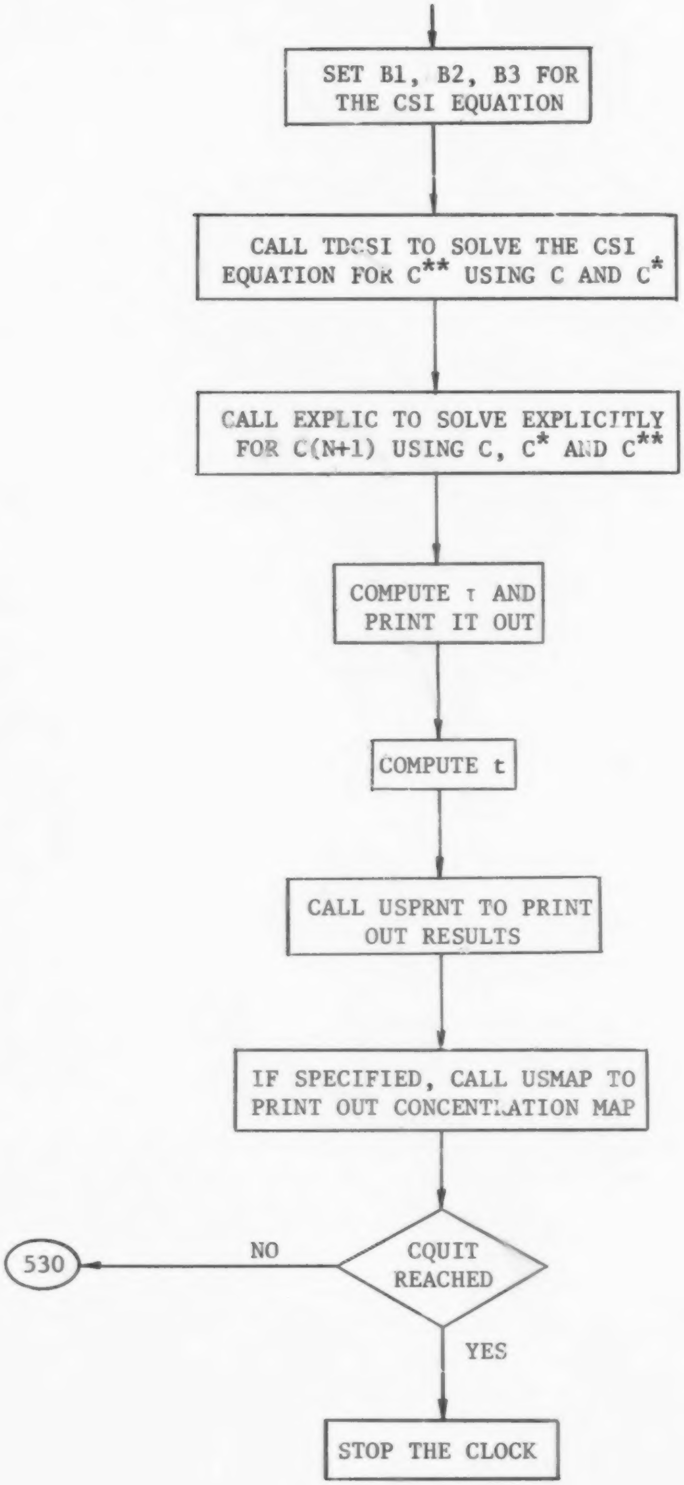
1 10	11 13	14 16
CQUIT	IQUIT	JQUIT

FLOW CHART OF MAIN - 2F2D

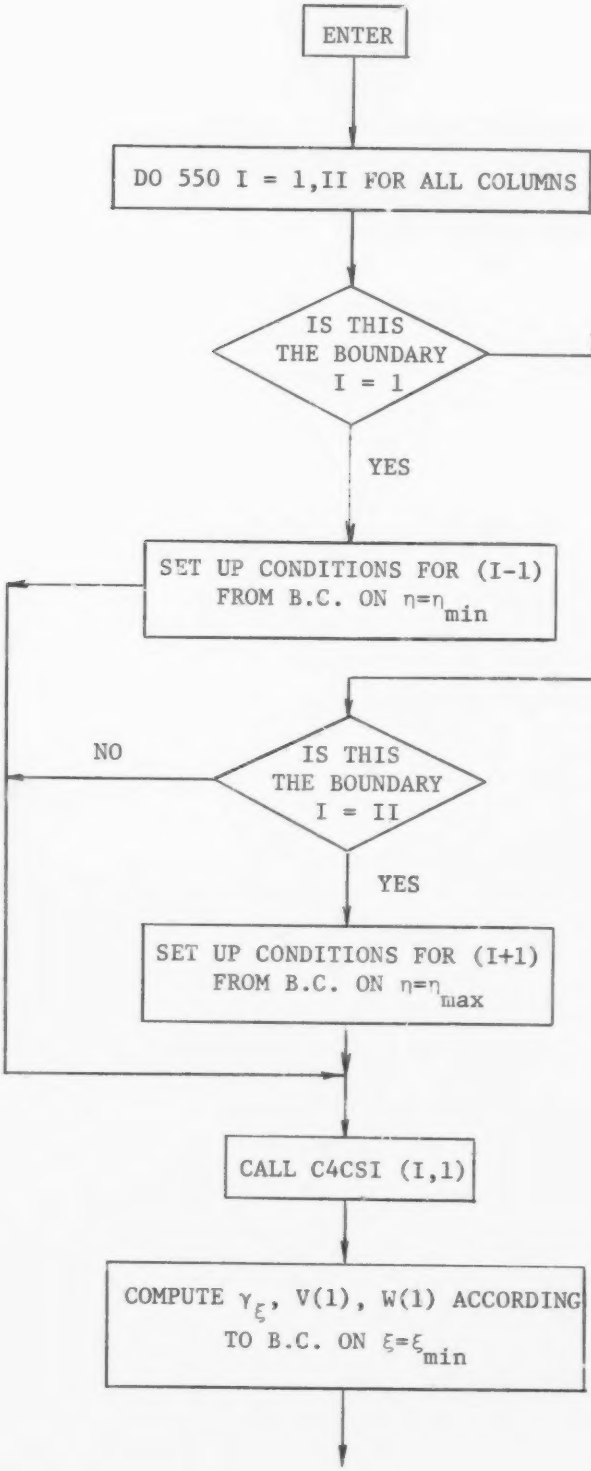

5
RESET CLOCK
READ AND PRINT DATA
COMPUTE THE NON-DIMENSIONAL QUANTITIES AND PRINT THEM OUT
INITIALIZE C, C^*, AND C^{**} TO ZERO
CALL SUBROUTINE CINPUT TO SET BOUNDARY CONDITION FOR $\eta=\eta_{min}$
COMPUTE FIRST TIME STEP $\Delta\tau$ = DTMIN$\cdot\Delta\eta$
SCHEME OPTION
=1
=2
=3
120
240
400
ONE EQUATION SCHEME
TWO EQUATION SCHEME
THREE EQUATION SCHEME
STOP THE CLOCK AND PRINT OUT COMPUTER TIME USED
GO TO 5

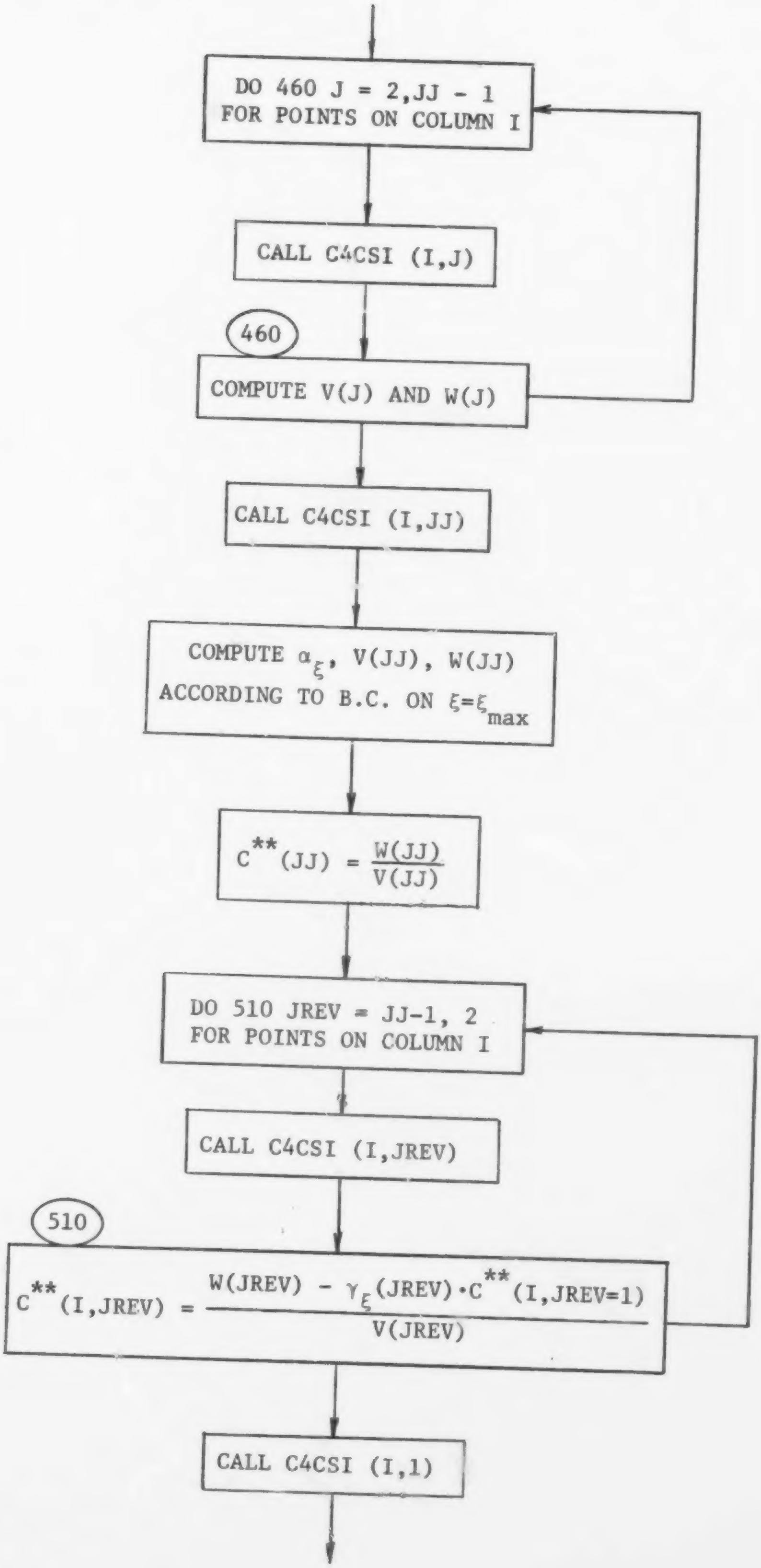
THREE EQUATION SCHEME

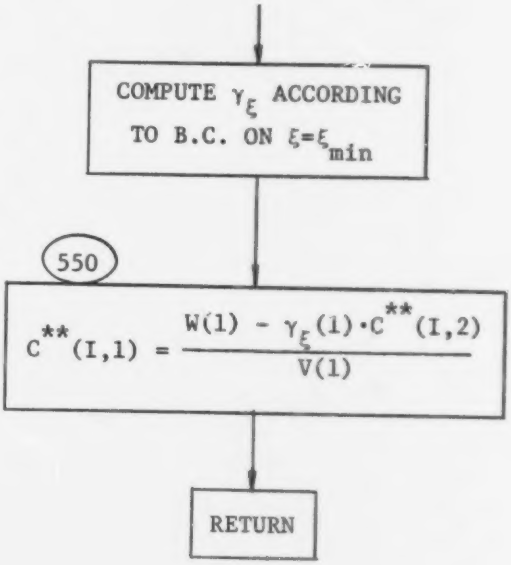

ISO = 3
DO 530 L = 1,NN
530
COMPUTE THE PRESENT Δτ
SAVE C(N) BY STORING IT IN C**
DIVIDE Δτ BY NCYC
SET B1, B2, B3 FOR THE ETA EQUATION
CALL TDETA TO SOLVE THE ETA EQUATIONS FOR C* USING C
DO 470 KK = 1,NCYC
LAST CYCLE
YES
NO
STORE MOST RECENT C* IN C FOR USE IN NEXT CYCLE
RESTORE C TO C(N) FROM TEMPORARY STORAGE IN C**
MULTIPLY Δτ BY NCYC


SET B1, B2, B3 FOR THE CSI EQUATION
CALL TDCSI TO SOLVE THE CSI EQUATION FOR C^{**} USING C AND C^{*}
CALL EXPLIC TO SOLVE EXPLICITLY FOR C(N+1) USING C, C^{*} AND C^{**}
COMPUTE τ AND PRINT IT OUT
COMPUTE t
CALL USPRNT TO PRINT OUT RESULTS
IF SPECIFIED, CALL USMAP TO PRINT OUT CONCENTRATION MAP
CQUIT REACHED
NO
530
YES
STOP THE CLOCK

FLOW CHART OF TDCSI


ENTER
DO 550 I = 1,II FOR ALL COLUMNS
IS THIS THE BOUNDARY I = 1
NO
YES
SET UP CONDITIONS FOR (I-1) FROM B.C. ON $\eta=\eta_{min}$
NO
IS THIS THE BOUNDARY I = II
YES
SET UP CONDITIONS FOR (I+1) FROM B.C. ON $\eta=\eta_{max}$
CALL C4CSI (I,1)
COMPUTE γ_ξ, V(1), W(1) ACCORDING TO B.C. ON $\xi=\xi_{min}$


DO 460 J = 2,JJ - 1
FOR POINTS ON COLUMN I
CALL C4CSI (I,J)
460
COMPUTE V(J) AND W(J)
CALL C4CSI (I,JJ)
COMPUTE α_ξ, V(JJ), W(JJ)
ACCORDING TO B.C. ON $\xi=\xi_{max}$
$C^{**}(JJ) = \frac{W(JJ)}{V(JJ)}$
DO 510 JREV = JJ-1, 2
FOR POINTS ON COLUMN I
CALL C4CSI (I,JREV)
510
$C^{**}(I,JREV) = \frac{W(JREV) - \gamma_\xi(JREV) \cdot C^{**}(I,JREV=1)}{V(JREV)}$
CALL C4CSI (I,1)


COMPUTE γ_ξ ACCORDING TO B.C. ON $\xi=\xi_{min}$
550
$C^{**}(I,1) = \frac{W(1) - \gamma_\xi(1)\cdot C^{**}(I,2)}{V(1)}$
RETURN

```
*     M3880-3232,FMS,DEBUG,5,5,10000,0                                  1F1D
*     SYMBOL TABLE                                                      1F1D
*     XEQ                                                               1F1D
*     LABEL                                                             1F1D
C     1F1D=1-DIM FLOW WITH 1-DIM DISPERSION.                            1F1D
C***********************  SYMBOLS USED  ********************************1F1D
C     A1-A4= WEIGHTING COEFFICIENTS IN THE CONVECTIVE TERM.             1F1D
C     B1-B3= WEIGHTING COEFFICIENTS IN THE TIME TERM.                   1F1D
C     CFBC= B.C. ON X=0.                                                1F1D
C     CLBC=B.C. ON X=EL.                                                1F1D
C     CQUIT= VALUE OF C AT IQUIT WHICH TERMINATES THE CALCULATION.      1F1D
C     D= LONGITUDINAL DISPERSION COEFFICIENT.                           1F1D
C     DT= TIME STEP (VARIABLE).                                         1F1D
C     DTMAX= LARGEST VALUE OF VEL*DT/DX.                                1F1D
C     DTMIN= INITIAL VALUE OF VEL*DT/DX.                                1F1D
C     DTSTEP= MULTIPLIER FOR SUCCESSIVE TIME INCREMENTS.                1F1D
C     DX= SPACE INCREMENT.                                              1F1D
C     ECN= WEIGHTING COEFFICIENT IN SECOND DERIVATIVE (CRANK-NICHOLSON) 1F1D
C     EL= LENGTH OF MEDIA.                                              1F1D
C     EPS= WEIGHTING COEFFICIENT IN CONVECTIVE TERM.                    1F1D
C     FTETA(I)= VALUE OF TETA IN I-TH CYCLE.                            1F1D
C     II= NUMBER OF GRID POINTS.                                        1F1D
C     IQUIT= POINT AT WHICH CQUIT TERMINATES THE CALCULATION.           1F1D
C     JFBC= TYPE B.C. ON X=0.                                           1F1D
C     JLBC= TYPE B.C. ON X=EL.                                          1F1D
C     NCYCLE= NUMBER OF CYCLES.                                         1F1D
C     NDIV= NUMBER OF SLICES ON X=0 TO X=EL.                            1F1D
C     NN= NUMBER OF TIME STEPS TO BE TAKEN.                             1F1D
C     VEL= SEEPAGE VELOCITY.                                            1F1D
C                                                                       1F1D
      DIMENSION C(503),CSTAR(503),FTETA(5)                              1F1D
      COMMON II,C,CSTAR,T,TETA,DT,D,DX,VEL,JFBC,CFBC,JLBC,CLBC,ECN,     1F1D
     1A1,A2,A3,A4,B1,B2,B3,ZETA,BETA,GAMA,DELTA1,DELTA2,DELTA3,VAR,NR   1F1D
    5 CALL RSCLCK                                                       1F1D
   10 READ 1000,NDIV,EL,VEL,D                                           1F1D
 1000 FORMAT (I5,3F10.5)                                                1F1D
      READ 1000,NN,DTMAX                                                1F1D
      READ 1001,EPS,ECN                                                 1F1D
      READ 1001,DTSTEP,DTMIN                                            1F1D
 1001 FORMAT (2F10.5)                                                   1F1D
      READ 1000,IQUIT,CQUIT                                             1F1D
      READ 1002,JFBC,CFBC,JLBC,CLBC                                     1F1D
 1002 FORMAT (I3,F7.2,I3,F7.2)                                          1F1D
      READ 1000,NCYCLE,(FTETA(I),I=1,3)                                 1F1D
      DX=EL/FLOATF(NDIV)                                                1F1D
      II=NDIV+1                                                         1F1D
      DT=DTMIN*DX/VEL                                                   1F1D
      PRINT 2000,NCYCLE                                                 1F1D
 2000 FORMAT(21H1ONE DIM. DISPERSION,,I3,14H EQS PER CYCLE)             1F1D
      PRINT 2001,EL,VEL,D                                               1F1D
 2001 FORMAT(3H L=F7.2,3H V=F7.2,3H D=F7.4)                             1F1D
      PRINT 2002,NN,DTMAX                                               1F1D
 2002 FORMAT (1H ,I3,6H STEPS,16H (VEL*DT/DX)MAX=F7.2)                  1F1D
      PRINT 2003,((I,FTETA(I)),I=1,NCYCLE)                              1F1D
 2003 FORMAT(3(6H TETA(,I1,2H)=F7.4))                                   1F1D
```

```
      PRINT 2004,EPS                                                    1F1D
 2004 FORMAT(5H EPS=F7.4)                                               1F1D
      PRINT 2005,JFBC,CFBC,JLBC,CLBC                                    1F1D
 2005 FORMAT(6H JFBC=I3,6H CFBC=F7.2,6H JLBC=I3,6H CLBC=F7.2)           1F1D
      PRINT 2006,NDIV,DX,DT                                             1F1D
 2006 FORMAT(1H ,I4,7H SLICES,4H DX=F7.5,10H FIRST DT=F7.5)             1F1D
      PRINT 2007,ECN                                                    1F1D
 2007 FORMAT (9H C-N EPS=F7.4)                                          1F1D
      DO 20 I=1,II                                                      1F1D
      C(I)=0.                                                           1F1D
   20 CSTAR(I)=0.                                                       1F1D
      DT=DT/DTSTEP                                                      1F1D
   25 T=0.                                                              1F1D
      A1=0.5*(1.-EPS)                                                   1F1D
      A4=A1                                                             1F1D
      A2=0.5*EPS                                                        1F1D
      A3=A2                                                             1F1D
      DO 30 N=1,NN                                                      1F1D
      DARG=DT*VEL/DX                                                    1F1D
      IF (DARG-DTMAX) 100,120,120                                       1F1D
  100 DT=DT*DTSTEP                                                      1F1D
      DARG=DT*VEL/DX                                                    1F1D
      IF (DARG-DTMAX) 120,120,110                                       1F1D
  110 DT=DTMAX*DX/VEL                                                   1F1D
  120 DT=DT/FLOATF(NCYCLE)                                              1F1D
      DO 40 K=1,NCYCLE                                                  1F1D
      TETA=FTETA(K)                                                     1F1D
      B1=1.-TETA                                                        1F1D
      B2=0.5*TETA                                                       1F1D
      B3=B2                                                             1F1D
      DO 50 I=1,II                                                      1F1D
   50 CSTAR(I)=C(I)                                                     1F1D
   40 CALL TD1DIM                                                       1F1D
      DT=DT*FLOATF(NCYCLE)                                              1F1D
      T=T+DT                                                            1F1D
      CALL USOUTP                                                       1F1D
      CALL USEX1(EL,VEL,D,T)                                            1F1D
   70 IF (C(IQUIT)-CQUIT) 30,80,80                                      1F1D
   30 CONTINUE                                                          1F1D
   80 CALL STOPCL(KCT)                                                  1F1D
      PRINT 5000,KCT                                                    1F1D
 5000 FORMAT(15H COMPUTER TIME=I10,19H 60THS OF A SECOND.)              1F1D
      GO TO 5                                                           1F1D
      END                                                               1F1D
```

```
      SUBROUTINE TD1DIM                                                 TD1DIM
*     SYMBOL TABLE                                                      TD1DIM
*     LABEL                                                             TD1DIM
*     LIST 8                                                            TD1DIM
C     TD2DIM, FEB. 22, 1966.                                            TD1DIM
C     TD1DIM= TRI-DIAGONAL SOLVER FOR THE 1-DIMENSIONAL CASE.           TD1DIM
```

```
      DIMENSION C(503),CSTAR(503),V(503),W(503)                          TD1DIM
      COMMON II,C,CSTAR,T,TETA,DT,D,DX,VEL,JFBC,CFBC,JLBC,CLBC,ECN,      TD1DIM
     1A1,A2,A3,A4,B1,B2,B3,ZETA,BETA,GAMA,DELTA1,DELTA2,DELTA3            TD1DIM
      GO TO (10,20,30),JFBC                                              TD1DIM
   10 CALL C4TD1D(1)                                                     TD1DIM
      GFC=GAMA+ZETA                                                      TD1DIM
      W(1)=(DELTA3+DELTA1)*CSTAR(2)+DELTA2*CSTAR(1)                      TD1DIM
      V(1)=BETA                                                          TD1DIM
      IB=2                                                               TD1DIM
      GO TO 40                                                           TD1DIM
   20 CALL C4TD1D(1)                                                     TD1DIM
      GFC=GAMA-ZETA                                                      TD1DIM
      W(1)=(DELTA3-DELTA1)*CSTAR(2)+(DELTA2+2.*DELTA1)*CSTAR(1)          TD1DIM
      V(1)=BETA+2.*ZETA                                                  TD1DIM
      IB=2                                                               TD1DIM
      GO TO 40                                                           TD1DIM
   30 CALL C4TD1D(2)                                                     TD1DIM
      GFC=GAMA                                                           TD1DIM
      W(2)=(DELTA1-ZETA)*CFBC+DELTA2*CSTAR(2)+DELTA3*CSTAR(3)            TD1DIM
      V(2)=BETA                                                          TD1DIM
      IB=3                                                               TD1DIM
   40 IIM1=II-1                                                          TD1DIM
      DO 50 I=IB,IIM1                                                    TD1DIM
      CALL C4TD1D(I)                                                     TD1DIM
      V(I)=BETA-((ZETA*GFC)/V(I-1))                                      TD1DIM
      RHS=DELTA1*CSTAR(I-1)+DELTA2*CSTAR(I)+DELTA3*CSTAR(I+1)            TD1DIM
      W(I)=RHS-((ZETA*W(I-1))/V(I-1))                                    TD1DIM
   50 GFC=GAMA                                                           TD1DIM
      CALL C4TD1D(II)                                                    TD1DIM
      GO TO (60,70,80),JLBC                                              TD1DIM
   60 ZFC=ZETA+GAMA                                                      TD1DIM
      RHS=DELTA2*CSTAR(II)+(DELTA1+DELTA3)*CSTAR(II-1)                   TD1DIM
      V(II)=BETA                                                         TD1DIM
      GO TO 90                                                           TD1DIM
   70 ZFC=ZETA-GAMA                                                      TD1DIM
      RHS=(DELTA2+2.*DELTA3)*CSTAR(II)+(DELTA1-DELTA3)*CSTAR(II-1)       TD1DIM
      V(II)=BETA+2.*GAMA                                                 TD1DIM
      GO TO 90                                                           TD1DIM
   80 ZFC=ZETA                                                           TD1DIM
      RHS=DELTA1*CSTAR(II-1)+DELTA2*CSTAR(II)+(DELTA3-GAMA)*CLBC         TD1DIM
      V(II)=BETA                                                         TD1DIM
   90 V(II)=V(II)-(ZFC*GAMA/V(II-1))                                     TD1DIM
      W(II)=RHS-(ZFC*W(II-1)/V(II-1))                                    TD1DIM
      C(II)=W(II)/V(II)                                                  TD1DIM
      IIM2=II-2                                                          TD1DIM
      DO 100 I=1,IIM2                                                    TD1DIM
      IREV=II-I                                                          TD1DIM
      CALL C4TD1D(IREV)                                                  TD1DIM
  100 C(IREV)=(W(IREV)-GAMA*C(IREV+1))/V(IREV)                           TD1DIM
      GO TO (110,120,130),JFBC                                           TD1DIM
  110 CALL C4TD1D(1)                                                     TD1DIM
      GFC=GAMA+ZETA                                                      TD1DIM
      C(1)=(W(1)-GFC*C(2))/V(1)                                          TD1DIM
      GO TO 140                                                          TD1DIM
  120 CALL C4TD1D(1)                                                     TD1DIM
```

```
      GFC=GAMA-ZETA                                                     TD1DIM
      C(1)=(W(1)-GFC*C(2))/V(1)                                         TD1DIM
      GO TO 140                                                         TD1DIM
  130 C(1)=CFBC                                                         TD1DIM
  140 RETURN                                                            TD1DIM
      END                                                               TD1DIM



      SUBROUTINE C4TD1D(I)                                              C4TD1D1
*     LIST 8                                                            C4TD1D1
*     SYMBOL TABLE                                                      C4TD1D1
*     LABEL                                                             C4TD1D1
C     C4TD1D-1 IS FOR HOMOGENEOUS MEDIA.                                C4TD1D1
C     C4TD1D GIVES THE COEFFICIENTS FOR TD1DIM AT POINT I.              C4TD1D1
      DIMENSION C(503),CSTAR(503)                                       C4TD1D1
      COMMON II,C,CSTAR,T,TETA,DT,D,DX,VEL,JFBC,CFBC,JLBC,CLBC,ECN,     C4TD1D1
     1A1,A2,A3,A4,B1,B2,B3,ZETA,BETA,GAMA,DELTA1,DELTA2,DELTA3          C4TD1D1
      DXSQ=DX*DX                                                        C4TD1D1
      ZETA=B3/DT-ECN*D/DXSQ-A4*VEL/DX                                   C4TD1D1
      BETA=B1/DT+2.*ECN*D/DXSQ+(A4-A3)*VEL/DX                           C4TD1D1
      GAMA=B2/DT-ECN*D/DXSQ+A3*VEL/DX                                   C4TD1D1
      DELTA1=B3/DT+(1.-ECN)*D/DXSQ+A2*VEL/DX                            C4TD1D1
      DELTA2=B1/DT-2.*(1.-ECN)*D/DXSQ+(A1-A2)*VEL/DX                    C4TD1D1
      DELTA3=B2/DT+(1.-ECN)*D/DXSQ-A1*VEL/DX                            C4TD1D1
      RETURN                                                            C4TD1D1
      END                                                               C4TD1D1



      SUBROUTINE USEX1(EL,VEL,D,T)                                      USEX1
*     SYMBOL TABLE                                                      USEX1
*     LABEL                                                             USEX1
C     USEX1 GIVES THE EXACT SOLUTION FOR LONG. DISP. AT TIME T.         USEX1
C     U. SHAMIR, JANUARY 5, 1966.                                       USEX1
      DIMENSION SOL(11),X(11)                                           USEX1
      DX=EL/10.                                                         USEX1
      X(1)=0.                                                           USEX1
      SOL(1)=1.0                                                        USEX1
      DO 10 I=2,11                                                      USEX1
      X(I)=FLOATF(I-1)*DX                                               USEX1
      ARG1=(X(I)-VEL*T)/(2.*SQRTF(D*T))                                 USEX1
      SOL(I)=0.5*(1.-ERRF(ARG1))                                        USEX1
      ARG2=(X(I)+VEL*T)/(2.*SQRTF(D*T))                                 USEX1
      IF (ABSF(ARG2)-4.) 10,10,20                                       USEX1
   20 US1=1./ARG2                                                       USEX1
      US2=-0.5/(ARG2**3)                                                USEX1
      US3=0.75/(ARG2**5)                                                USEX1
      US4=-1.875/(ARG2**7)                                              USEX1
      SUMU=US1+US2+US3+US4                                              USEX1
      SOL(I)=SOL(I)+0.2821*(EXPF(-ARG1*ARG1))*SUMU                      USEX1
   10 CONTINUE
      PRINT 1000,T
 1000 FORMAT(21H EXACT SOLUTION AT T=F15.5)
      PRINT 1001,(X(I),I=1,11)
 1001 FORMAT(3H X=,11F8.4)
      PRINT 1002,(SOL(I),I=1,11)
 1002 FORMAT(3H C=,11F8.4)
      RETURN
      END




      SUBROUTINE USOUTP
*     SYMBOL TABLE
*     LABEL
C     USOUTP IS A PRINTOUT S/R.
C     FOR THE ONE DIMENSIONAL CASE.
C     U. SHAMIR, DECEMBER 7, 1965.
      DIMENSION C(503),CSTAR(503)
      COMMON II,C,CSTAR,T,TETA,DT,D,DX,VEL,JFBC,CFBC,JLBC,CLBC,ECN,
     1A1,A2,A3,A4,B1,B2,B3,ZETA,BETA,GAMA,DELTA1,DELTA2,DELTA3
      PRINT 1000,T
 1000 FORMAT (26H RELATIVE CONC. C(J) AT T=F15.5,8H SECONDS)
      NN=II/5
      L=5*NN+1
      DO 10 N=1,NN
      K=5*(N-1)+1
      KK=K+4
   10 PRINT 1001,((I,C(I)),I=K,KK)
 1001 FORMAT (5(3H C(,I3,2H)=F10.5))
      IF (II-5*NN) 20,20,30
   30 PRINT 1001,((I,C(I)),I=L,II)
   20 RETURN
      END


C*****  NEED TO ADD SUBROUTINE ERRF  *********************
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*     M3880-3232,FMS,DEBUG,5,5,20000,0   2F2D30
*     XEQ                                                               2F2D
*     LABEL                                                             2F2D
*     SYMBOL TABLE                                                      2F2D
C     2F2D=2-DIM FLOW WITH 2-DIM DISPERSION IN NON-DIMENSIONAL          2F2D
C     FI-CSY COORDINATES (ETA AND CSI).                                 2F2D
C                                                                       2F2D
C***************************** SYMBOLS USED ****************************2F2D
C                                                                       2F2D
C     A1-A4= WEIGHTING COEFFICIENTS IN CONVECTIVE TERM.                 2F2D
C     ALFAL= LONGITUDINAL DISPERSIVITY.                                 2F2D
C     ALFALP= NON-DIMENSIONAL ALFAL.                                    2F2D
C     ALFAT= LATERAL DISPERSIVITY.                                      2F2D
C     ALFATP= NON-DIMENSIONAL ALFAT.                                    2F2D
C     B1-B3= WEIGHTING COEFFICIENTS IN TIME TERM.                       2F2D
C     CFCSI= B.C. FOR (I,0) STORED IN (I,JJ+1)                          2F2D
C     CFETA= B.C. FOR (0,J) STORED IN (II+1,J)                          2F2D
C     CLCSI= B.C. FOR (I,JJ) STORED IN (I,JJ+2)                         2F2D
C     CLETA= B.C. FOR (II,J) STORED IN (II+2,J)                         2F2D
C     CQUIT= VALUE OF CONCENTRATION AT REFERENCE POINT FOR TERMINATING. 2F2D
C     CSI= NON-DIMENSIONAL CSY.                                         2F2D
C     CSYNN AND CSYNX= LIMITS FOR CONCENTRATION INPUT.                  2F2D
C     DCSI= SPACE INCREMENT IN CSI DIRECTION.                           2F2D
C     DETA= SPACE INCREMENT IN ETA DIRECTION.                           2F2D
C     DMOL= MOLECULAR DIFFUSIVITY.                                      2F2D
C     DMOLP= NON-DIMENSIONAL DMOL.                                      2F2D
C     DTAU= INCREMENT OF TAU.                                           2F2D
C     DTMAX= MAXIMUM VALUE OF DTAU/DETA.                                2F2D
C     DTMIN= INITIAL VALUE OF DTUA/DETA.                                2F2D
C     DTSTEP= MULTIPLIER FOR SUCCESSIVE TIME INCREMENTS.                2F2D
C     ELZERO= REFERENCE LENGTH.                                         2F2D
C     ETA= NON-DIMENSIONAL FI.                                          2F2D
C     IDIV= NO. OF SLICES IN ETA DIRECTION FROM FIMIN TO FIMAX.         2F2D
C     II= NO. OF GRID POINTS IN ETA DIRECTION.                          2F2D
C     IMAP, NM= SIGNALS FOR MAP PRINTING (SEE SUBROUTINE USMAP)         2F2D
C     IPRNT, ISTEP, JSTEP= SIGNALS FOR PRINTING (SEE SUBROUTINE USPRNT) 2F2D
C     IQUIT, JQUIT= SUBSCRIPTS OF REFERENCE POINT.                      2F2D
C     ISO=1, ONE EQUATION, FOR LONGITUDINAL DISPERSION.                 2F2D
C     ISO=2, TWO IMPLICIT EQUATIONS.                                    2F2D
C     ISO=3, TWO IMPLICIT EQUATIONS AND ONE EXPLICIT EQUATION.          2F2D
C     JDIV= NO. OF SLICES IN CSI DIRECTION FROM CSYMIN TO CSYMAX.       2F2D
C     JJ= NO. OF GRID POINTS IN CSI DIRECTION.                          2F2D
C     K...=1 REFLECTION B.C.                                            2F2D
C     K..=2 TRNSMISSION B.C.                                            2F2D
C     K..=3 GIVEN B.C.                                                  2F2D
C     NCYC= NO. OF CYCLES IN ETA EQUATION.                              2F2D
C     NN= NO. OF TIME STEPS TO BE CALCULATED.                           2F2D
C     KIN= TYPE OF INPUT CONCENTRATION (SEE SUBROUTINE CINPUT)          2F2D
C     TAU= NON-DIMENSIONAL TIME.                                        2F2D
C     TETA(KK)= VARIABLE WEIGHTING COEFFICIENT FOR TIME TERM.           2F2D
C     UZERO= REFERENCE VELOCITY.                                        2F2D
C                                                                       2F2D
      DIMENSION C(53,53),CSTAR(53,53),CSS(53,53),TETA(3),TITLE(10)      2F2D
      COMMON C,CSTAR,CSS,II,JJ,DTAU,DETA,DCSI,ALFALP,ALFATP,DMOLP,      2F2D
     1UZERO,ELZERO,ETAMIN,CSIMIN,EPSAB,A1,A2,A3,A4,B1,B2,B3,            2F2D
     2KFETA,CFETA,KLETA,CLETA,KFCSI,CFCSI,KLCSI,CLCSI,                  2F2D
     3ZETAE,BETAE,GAMAE,DELTA1,DELTA2,DELTA3,DELTA4,DELTA5,             2F2D
     4ZETAC,BETAC,GAMAC,DELTA6,DELTA7,DELTA8,DELTA9,DELT10,RO1,RO2,RO3, 2F2D
     5ITABLE                                                            2F2D
      ITABLE=0                                                          2F2D
C     RESET CLOCK.                                                      2F2D
    5 CALL RSCLCK                                                       2F2D
C     READ  AND PRINT TITLE.                                            2F2D
      READ 9000,(TITLE(N),N=1,10)                                       2F2D
 9000 FORMAT(10A6)                                                      2F2D
      PRINT 9001,(TITLE(N),N=1,10)                                      2F2D
 9001 FORMAT(1H1,10A6///)                                               2F2D
C     READ AND PRINT SCHEME OPTION.                                     2F2D
      READ 1000,ISO                                                     2F2D
      GO TO (6,7,8),ISO                                                 2F2D
    6 PRINT 9002,ISO                                                    2F2D
 9002 FORMAT(14H SCHEME OPTION,I5,19H ONLY ETA EQUATION.)               2F2D
      GO TO 10                                                          2F2D
    7 PRINT 9003,ISO                                                    2F2D
 9003 FORMAT(14H SCHEME OPTION,I5,15H TWO EQUATIONS.)                   2F2D
      GO TO 10                                                          2F2D
    8 PRINT 9004,ISO                                                    2F2D
 9004 FORMAT(14H SCHEME OPTION,I5,29H THREE EQUATIONS=FULL SCHEME.)     2F2D
C     SIZE AND NUMBER OF SLICES IN ETA DIRECTION.                       2F2D
   10 READ 1000,IDIV,FIMIN,FIMAX                                        2F2D
 1000 FORMAT(I5,3F10.5)                                                 2F2D
      PRINT 2000,FIMIN,FIMAX,IDIV                                       2F2D
 2000 FORMAT(//4H FI=F10.5,7H TO FI=F10.5,I5,7H SLICES)                 2F2D
C     SIZE AND NUMBER OF SLICES IN CSY DIRECTION.                       2F2D
      READ 1000,JDIV,CSYMIN,CSYMAX                                      2F2D
      PRINT 2001,CSYMIN,CSYMAX,JDIV                                     2F2D
 2001 FORMAT (5H CSY=F10.5,8H TO CSY=F10.5,I5,7H SLICES)                2F2D
C     REFERENCE VALUES UZERO AND ELZERO.                                2F2D
      READ 1001,UZERO,ELZERO                                            2F2D
 1001 FORMAT(5F10.5)                                                    2F2D
      PRINT 2002,UZERO,ELZERO                                           2F2D
 2002 FORMAT (7H UZERO=F10.5,8H ELZERO=F10.5)                           2F2D
C     DISPERSIVITY COEFFICIENTS (LONG. LAT. AND MOLECULAR).             2F2D
      READ 1001,ALFAL,ALFAT,DMOL                                        2F2D
      PRINT 2003,ALFAL,ALFAT,DMOL                                       2F2D
 2003 FORMAT (7H ALFAL=F10.5,7H ALFAT=F10.5,6H DMOL=F10.5)              2F2D
C     BOUNDARY CONDITIONS.                                              2F2D
      READ 1002,KFETA,CFETA,KLETA,CLETA                                 2F2D
      READ 1002,KFCSI,CFCSI,KLCSI,CLCSI                                 2F2D
 1002 FORMAT (2(I3,F7.2))                                               2F2D
      PRINT 2004,KFETA,CFETA,KLETA,CLETA                                2F2D
 2004 FORMAT (7H KFETA=I3,7H CFETA=F7.2,7H KLETA=I3,7H CLETA=F7.2)      2F2D
      PRINT 2005,KFCSI,CFCSI,KLCSI,CLCSI                                2F2D
 2005 FORMAT (7H KFCSI=I3,7H CFCSI=F7.2,7H KLCSI=I3,7H CLCSI=F7.2)      2F2D
C     CONVECTIVE TERM WEIGHTING COEFFICIENTS.                           2F2D
      READ 1001,A1,A2,A3,A4                                             2F2D
      PRINT 2006,A1,A2,A3,A4                                            2F2D
 2006 FORMAT(4H A1=F10.5,4H A2=F10.5,4H A3=F10.5,4H A4=F10.5)           2F2D
C     NUMBER OF CYCLES PER TIME STEP AND TETA(I).                       2F2D
      READ 1000,NCYC,(TETA(I),I=1,NCYC)                                 2F2D
      PRINT 2007,NCYC,(TETA(I),I=1,NCYC)                                2F2D
 2007 FORMAT (1H ,I3,16H CYCLES TETA(I)=,3F10.5)                        2F2D
C     TIME STEP SEQUENCE (NUMBER OF STEPS, MIN,MAX,STEP)                2F2D
      READ 1000,NN,DTMIN,DTMAX,DTSTEP                                   2F2D
      PRINT 2008,NN,DTMIN,DTMAX,DTSTEP                                  2F2D
 2008 FORMAT(1H ,I5,14H STEPS, DTMIN=F10.5,7H DTMAX=F10.5,              2F2D
     18H DTSTEP=F10.5)                                                  2F2D
C     INPUT CONCENTRATION (TYPE,FROM CSY=CSYNN TO CSY=CSYNX)            2F2D
      READ 1000,KIN,CSYNN,CSYNX                                         2F2D
      PRINT 2009,KIN,CSYNN,CSYNX                                        2F2D
 2009 FORMAT (5H KIN=I3,10H FROM CSY=F7.2,8H TO CSY=F7.2)               2F2D
C     IMAP=1 PRINT MAP EVERY NM STEPS.                                  2F2D
C     IMAP=2 DO NOT PRINT MAPS.                                         2F2D
      READ 1003,IMAP,NM                                                 2F2D
 1003 FORMAT (3I3)                                                      2F2D
C     IPRNT=1 PRINT OUT THE WHOLE ARRAY.                                2F2D
C     IPRNT=2 PRINT OUT ONLY EVERY ISTEP IN ETA AND JSTEP IN CSI.       2F2D
      READ 1003,IPRNT,ISTEP,JSTEP                                       2F2D
C     CONCENTRATION VALUE FOR TERMINATING THE CALCULATION.              2F2D
C     (VALUE, I AND J OF POINT)                                         2F2D
      READ 1004,CQUIT,IQUIT,JQUIT                                       2F2D
 1004 FORMAT (F10.5,2I3)                                                2F2D
C     COMPUTE NON-DIMENSIONAL QUANTITIES.                               2F2D
      DENOM=UZERO*ELZERO                                                2F2D
      ETAMIN=FIMIN/DENOM                                                2F2D
      ETAMAX=FIMAX/DENOM                                                2F2D
      CSIMIN=CSYMIN/DENOM                                               2F2D
      CSIMAX=CSYMAX/DENOM                                               2F2D
      CSINN=CSYNN/DENOM                                                 2F2D
      CSINX=CSYNX/DENOM                                                 2F2D
      ALFALP=ALFAL/ELZERO                                               2F2D
      ALFATP=ALFAT/ELZERO                                               2F2D
      DMOLP=DMOL/DENOM                                                  2F2D
C     SPACE INCREMENTS.                                                 2F2D
      DETA=(ETAMAX-ETAMIN)/FLOATF(IDIV)                                 2F2D
      IF (JDIV) 11,11,12                                                2F2D
   11 DCSI=0.0                                                          2F2D
      GO TO 13                                                          2F2D
   12 DCSI=(CSIMAX-CSIMIN)/FLOATF(JDIV)                                 2F2D
C     PRINT OUT NON DIMENSIONAL QUANTITIES.                             2F2D
   13 PRINT 2010                                                        2F2D
 2010 FORMAT(//30H    NON-DIMENSIONAL QUANTITIES//)                     2F2D
      PRINT 2011,ETAMIN,ETAMAX,DETA                                     2F2D
 2011 FORMAT(10H FROM ETA=F10.5,8H TO ETA=F10.5,15H WITH STEPS OF F10.5)2F2D
      PRINT 2012,CSIMIN,CSIMAX,DCSI                                     2F2D
 2012 FORMAT(10H FROM CSI=F10.5,8H TO CSI=F10.5,15H WITH STEPS OF F10.5)2F2D
      PRINT 2013,ALFALP,ALFATP,DMOLP                                    2F2D
 2013 FORMAT (8H ALFALP=F10.5,8H ALFATP=F10.5,7H DMOLP=F10.5)           2F2D
C     NUMBER OF GRID POINTS IN ETA DIRECTION.                           2F2D
      II=IDIV+1                                                         2F2D
C     NUMBER OF GRID POINTS IN CSI DIRECTION.                           2F2D
      JJ=JDIV+1                                                         2F2D
C     INITIALIZE TO ZERO (INCLUDING B.C.).                              2F2D
      IIP2=II+2                                                         2F2D
      JJP2=JJ+2                                                         2F2D
      DO 100 I=1,IIP2                                                   2F2D
      DO 100 J=1,JJP2                                                   2F2D
      C(I,J)=0.                                                         2F2D
      CSTAR(I,J)=0.                                                     2F2D
  100 CSS(I,J)=0.                                                       2F2D
C     SET FIXED B.C. ON ETA=ETAMIN                                      2F2D
      CALL CINPUT(CSINN,CSINX,KIN)                                      2F2D
C     FIRST TIME STEP.                                                  2F2D
      DTAU=DTMIN*DETA                                                   2F2D
      PRINT 2014,DTAU                                                   2F2D
 2014 FORMAT(22H FIRST TIME STEP DTAU=F10.7////)                        2F2D
  110 T=0.                                                              2F2D
      TAU=0.                                                            2F2D
      NP=0                                                              2F2D
      DTAU=DTAU/DTSTEP                                                  2F2D
      GO TO (120,240,400),ISO                                           2F2D
C                                                                       2F2D
C**************************** ONE EQUATION OPTION **********************2F2D
C                                                                       2F2D
  120 DO 220 L=1,NN                                                     2F2D
      DARG=DTAU/DETA                                                    2F2D
      IF (DARG-DTMAX) 130,150,150                                       2F2D
  130 DTAU=DTSTEP*DTAU                                                  2F2D
      DARG=DTAU/DETA                                                    2F2D
      IF (DARG-DTMAX) 150,140,140                                       2F2D
  140 DTAU=DTMAX*DETA                                                   2F2D
  150 CONTINUE                                                          2F2D
      DTAU=DTAU/FLOATF(NCYC)                                            2F2D
      DO 180 KK=1,NCYC                                                  2F2D
      B1=1.-TETA(KK)                                                    2F2D
      B2=0.5*TETA(KK)                                                   2F2D
      B3=B2                                                             2F2D
C     SOLVE THE ETA EQUATION FOR CSTAR.                                 2F2D
      CALL TDETA                                                        2F2D
C     A DUMMY STATEMENT FOR POSSIBLE DUMP OF TEMPORARY VALUES.           2F2D
  160 CONTINUE                                                          2F2D
C     STORE MOST RECENT RESULTS FOR CSTAR IN C FOR USE IN NEXT CYCLE.   2F2D
      DO 170 I=1,II                                                     2F2D
      DO 170 J=1,JJ                                                     2F2D
  170 C(I,J)=CSTAR(I,J)                                                 2F2D
  180 CONTINUE                                                          2F2D
      DTAU=DTAU*FLOATF(NCYC)                                            2F2D
      TAU=TAU+DTAU                                                      2F2D
      PRINT 2015,TAU                                                    2F2D
 2015 FORMAT(5H TAU=F10.5)                                              2F2D
      T=TAU*ELZERO/UZERO                                                2F2D
      CALL USPRNT(T,IPRNT,ISTEP,JSTEP)                                  2F2D
      GO TO (190,210),IMAP                                              2F2D
  190 NP=NP+1                                                           2F2D
      IF (NM-NP) 200,200,210                                            2F2D
  200 CALL USMAP(T)                                                     2F2D
      NP=0                                                              2F2D
  210 IF (C(IQUIT,JQUIT)-CQUIT) 220,230,230                             2F2D
  220 CONTINUE                                                          2F2D
  230 GO TO 550                                                         2F2D
```

```
C                                                                       2F2D
C**************************** TWO EQUATION OPTION **********************2F2D
C                                                                       2F2D
  240 DO 380 L=1,NN                                                     2F2D
      DARG=DTAU/DETA                                                    2F2D
      IF (DARG-DTMAX) 250,270,270                                       2F2D
  250 DTAU=DTSTEP*DTAU                                                  2F2D
      DARG=DTAU/DETA                                                    2F2D
      IF (DARG-DTMAX) 270,260,260                                       2F2D
  260 DTAU=DTMAX*DETA                                                   2F2D
  270 CONTINUE                                                          2F2D
      DTAU=DTAU/FLOATF(NCYC)                                            2F2D
C     SAVE C(N) BY STORING IN CSS.                                      2F2D
      DO 280 I=1,II                                                     2F2D
      DO 280 J=1,JJ                                                     2F2D
  280 CSS(I,J)=C(I,J)                                                   2F2D
      DO 310 KK=1,NCYC                                                  2F2D
      B1=1.-TETA(KK)                                                    2F2D
      B2=0.5*TETA(KK)                                                   2F2D
      B3=B2                                                             2F2D
C     SOLVE THE ETA EQUATIONS FOR CSTAR.                                2F2D
      CALL TDETA                                                        2F2D
C     A DUMMY STATEMENT FOR POSSIBLE DUMP OF INTERMEDIATE VALUES.       2F2D
  285 CONTINUE                                                          2F2D
      IF (NCYC-KK) 310,310,290                                          2F2D
C     STORE MOST RECENT RESULTS FOR CSTAR IN C TO BE USED IN NEXT CYCLE.2F2D
C                                                                       2F2D
  290 DO 300 I=1,II                                                     2F2D
      DO 300 J=1,JJ                                                     2F2D
  300 C(I,J)=CSTAR(I,J)                                                 2F2D
  310 CONTINUE                                                          2F2D
C     RESTORE C TO C(N) FROM TEMPORARY STORAGE IN CSS.                  2F2D
      DO 320 I=1,II                                                     2F2D
      DO 320 J=1,JJ                                                     2F2D
  320 C(I,J)=CSS(I,J)                                                   2F2D
      DTAU=DTAU*FLOATF(NCYC)                                            2F2D
C     WEIGHTING COEFFICIENTS IN TIME TERM FOR THE CSI EQUATION.         2F2D
      B1=0.6667                                                         2F2D
      B2=0.1667                                                         2F2D
      B3=B2                                                             2F2D
C     SOLVE THE CSI EQUATIONS FOR CSS.                                  2F2D
      CALL TDCSI                                                        2F2D
C     A DUMMY STATEMENT FOR POSSIBLE DUMP OF INTERMEDIATE VALUES.       2F2D
  330 CONTINUE                                                          2F2D
C     COPY C(N+1) FROM CSS.                                             2F2D
      DO 340 I=1,II                                                     2F2D
      DO 340 J=1,JJ                                                     2F2D
  340 C(I,J)=CSS(I,J)                                                   2F2D
      TAU=TAU+DTAU                                                      2F2D
      PRINT 2015,TAU                                                    2F2D
      T=TAU*ELZERO/UZERO                                                2F2D
      CALL USPRNT(T,IPRNT,ISTEP,JSTEP)                                  2F2D
      GO TO (350,370),IMAP                                              2F2D
  350 NP=NP+1                                                           2F2D
      IF (NM-NP) 360,360,370                                            2F2D
  360 CALL USMAP(T)                                                     2F2D
      NP=0                                                              2F2D
  370 IF (C(IQUIT,JQUIT)-CQUIT) 380,390,390                             2F2D
  380 CONTINUE                                                          2F2D
  390 GO TO 550                                                         2F2D
C                                                                       2F2D
C**************************** THREE EQUATION OPTION ********************2F2D
C                                                                       2F2D
  400 DO 530 L=1,NN                                                     2F2D
      DARG=DTAU/DETA                                                    2F2D
      IF (DARG-DTMAX) 410,430,430                                       2F2D
  410 DTAU=DTSTEP*DTAU                                                  2F2D
      DARG=DTAU/DETA                                                    2F2D
      IF (DARG-DTMAX) 430,420,420                                       2F2D
  420 DTAU=DTMAX*DETA                                                   2F2D
  430 CONTINUE                                                          2F2D
      DTAU=DTAU/FLOATF(NCYC)                                            2F2D
C     SAVE C(N) BY STORING IN CSS.                                      2F2D
      DO 440 I=1,II                                                     2F2D
      DO 440 J=1,JJ                                                     2F2D
  440 CSS(I,J)=C(I,J)                                                   2F2D
      DO 470 KK=1,NCYC                                                  2F2D
      B1=1.-TETA(KK)                                                    2F2D
      B2=0.5*TETA(KK)                                                   2F2D
      B3=B2                                                             2F2D
C     SOLVE THE ETA EQUATIONS FOR CSTAR.                                2F2D
      CALL TDETA                                                        2F2D
C     A DUMMY STATEMENT FOR POSSIBLE DUMP OF INTERMEDIATE VALUES.      2F2D
  445 CONTINUE                                                          2F2D
      IF (NCYC-KK) 470,470,450                                          2F2D
C     STORE MOST RECENT RESULTS FOR CSTAR IN C TO BE USED IN NEXT CYCLE.2F2D
  450 DO 460 I=1,II                                                     2F2D
      DO 460 J=1,JJ                                                     2F2D
  460 C(I,J)=CSTAR(I,J)                                                 2F2D
  470 CONTINUE                                                          2F2D
C     RESTORE C TO C(N) FROM TEMPORARY STORAGE IN CSS.                  2F2D
      DO 480 I=1,II                                                     2F2D
      DO 480 J=1,JJ                                                     2F2D
  480 C(I,J)=CSS(I,J)                                                   2F2D
      DTAU=DTAU*FLOATF(NCYC)                                            2F2D
C     WEIGHTING COEFFICIENTS FOR THE TIME TERM IN THE CSI EQUATION.    2F2D
      B1=0.6667                                                         2F2D
      B2=0.1667                                                         2F2D
      B3=B2                                                             2F2D
C     SOLVE THE CSI EQUATIONS FOR CSS.                                  2F2D
      CALL TDCSI                                                        2F2D
C     A DUMMY STATEMENT FOR POSSIBLE DUMP OF INTERMEDIATE VALUES.      2F2D
  490 CONTINUE                                                          2F2D
C     SOLVE EXPLICITELY FOR C(N+1).                                     2F2D
      CALL EXPLIC                                                       2F2D
      TAU=TAU+DTAU                                                      2F2D
      PRINT 2015,TAU                                                    2F2D
      T=TAU*ELZERO/UZERO                                                2F2D
      CALL USPRNT(T,IPRNT,ISTEP,JSTEP)                                  2F2D
      GO TO (500,520),IMAP                                              2F2D
  500 NP=NP+1                                                          2F2D
      IF (NM-NP) 510,510,520                                           2F2D
  510 CALL USMAP(T)                                                    2F2D
      NP=0                                                             2F2D
  520 IF (C(IQUIT,JQUIT)-CQUIT) 530,540,540                            2F2D
  530 CONTINUE                                                         2F2D
  540 CONTINUE                                                         2F2D
C     STOP THE CLOCK, AND PRINT OUT COMPUTER TIME USED.                2F2D
  550 CALL STOPCL(KCT)                                                 2F2D
      PRINT 9010, KCT                                                  2F2D
 9010 FORMAT(15H COMPUTER TIME=I15,19H 60THS OF A SECOND.)             2F2D
      GO TO 5                                                          2F2D
      END                                                              2F2D
```

```
      SUBROUTINE TDETA                                                 TDETA
*     LABEL                                                            TDETA
*     SYMBOL TABLE                                                     TDETA
C     TDETA SOLVES THE TRI-DIAGONAL MATRIX OF THE ETA-EQUATION         TDETA
C     FOR CSTAR USING C.                                               TDETA
      DIMENSION C(53,53),CSTAR(53,53),CSS(53,53),V(53),W(53)           TDETA
      COMMON C,CSTAR,CSS,II,JJ,DTIME,DETA,DCSI,ALFALP,ALFATP,DMOLP,    TDETA
     1UZERO,ELZERO,ETAMIN,CSIMIN,EPSAB,A1,A2,A3,A4,B1,B2,B3,           TDETA
     2KFETA,CFETA,KLETA,CLETA,KFCSI,CFCSI,KLCSI,CLCSI,                 TDETA
     3ZETAE,BETAE,GAMAE,DELTA1,DELTA2,DELTA3,DELTA4,DELTA5,            TDETA
     4ZETAC,BETAC,GAMAC,DELTA6,DELTA7,DELTA8,DELTA9,DELT10,RO1,RO2,RO3 TDETA
      SUMF(S1,P1,S2,P2,S3,P3,S4,P4,S5,P5)=S1*P1+S2*P2+S3*P3+S4*P4+S5*P5 TDETA
      DO 280 J=1,JJ                                                    TDETA
      IF (J-1) 30,30,40                                                TDETA
   30 JM1=2                                                            TDETA
      GO TO (50,60,70),KFCSI                                           TDETA
   50 SIGM=1.                                                          TDETA
      SM=0.                                                            TDETA
      GO TO 100                                                        TDETA
   60 SIGM=-1.                                                         TDETA
      SM=2.                                                            TDETA
      GO TO 100                                                        TDETA
   70 SIGM=1.                                                          TDETA
      SM=0.                                                            TDETA
      JM1=JJ+1                                                         TDETA
      GO TO 100                                                        TDETA
   40 JM1=J-1                                                          TDETA
      SIGM=1.                                                          TDETA
      SM=0.                                                            TDETA
      IF (JJ-J) 90,90,100                                              TDETA
   90 JP1=JJ-1                                                         TDETA
      GO TO (110,120,130),KLCSI                                        TDETA
  110 SIGP=1.                                                          TDETA
      SP=0.                                                            TDETA
      GO TO 140                                                        TDETA
  120 SIGP=-1.                                                         TDETA
      SP=2.                                                            TDETA
      GO TO 140                                                         TDETA
  130 SIGP=1.                                                           TDETA
      SP=0.                                                             TDETA
      JP1=JJ+2                                                          TDETA
      GO TO 140                                                         TDETA
  100 JP1=J+1                                                           TDETA
      SIGP=1.                                                           TDETA
      SP=0.                                                             TDETA
  140 CIJ=C(1,J)                                                        TDETA
      CIP1J=C(2,J)                                                      TDETA
      CALL C4ETA(1,J)                                                   TDETA
      GO TO (150,160,170),KFETA                                         TDETA
  150 CIM1J=C(2,J)                                                      TDETA
      GFC=GAMAE+ZETAE                                                   TDETA
      V(1)=BETAE                                                        TDETA
      W(1)=0.                                                           TDETA
      GO TO 180                                                         TDETA
  160 CIM1J=-C(2,J)+2.*C(1,J)                                           TDETA
      GFC=GAMAE-ZETAE                                                   TDETA
      V(1)=BETAE+2.*ZETAE                                               TDETA
      W(1)=0.                                                           TDETA
      GO TO 180                                                         TDETA
  170 CIM1J=C(II+1,J)                                                   TDETA
      GFC=GAMAE                                                         TDETA
      V(1)=BETAE                                                        TDETA
      W(1)=-ZETAE*CSTAR(II+1,J)                                         TDETA
  180 CIJM1=SIGM*C(1,JM1)+SM*C(1,1)                                     TDETA
      CIJP1=SIGP*C(1,JP1)+SP*C(1,JJ)                                    TDETA
      W(1)=W(1)+SUMF(DELTA1,CIM1J,DELTA2,CIJ,DELTA3,CIP1J,DELTA4,CIJM1, TDETA
     1DELTA5,CIJP1)                                                     TDETA
      IIM1=II-1                                                         TDETA
      DO 190 I=2,IIM1                                                   TDETA
      CALL C4ETA(I,J)                                                   TDETA
      V(I)=BETAE-(GFC*ZETAE)/V(I-1)                                     TDETA
      CIJ=C(I,J)                                                        TDETA
      CIM1J=C(I-1,J)                                                    TDETA
      CIP1J=C(I+1,J)                                                    TDETA
      CIJM1=SIGM*C(I,JM1)+SM*C(I,1)                                     TDETA
      CIJP1=SIGP*C(I,JP1)+SP*C(I,JJ)                                    TDETA
      RHS=SUMF(DELTA1,CIM1J,DELTA2,CIJ,DELTA3,CIP1J,DELTA4,CIJM1,       TDETA
     1DELTA5,CIJP1)                                                     TDETA
      W(I)=RHS-(W(I-1)*ZETAE)/V(I-1)                                    TDETA
  190 GFC=GAMAE                                                         TDETA
      I=II                                                              TDETA
      CALL C4ETA (II,J)                                                 TDETA
      GO TO (200,210,220),KLETA                                         TDETA
  200 CIP1J=C(II-1,J)                                                   TDETA
      AFC=ZETAE+GAMAE                                                   TDETA
      V(II)=BETAE                                                       TDETA
      W(II)=0.                                                          TDETA
      GO TO 230                                                         TDETA
  210 CIP1J=-C(II-1,J)+2.*C(II,J)                                       TDETA
      AFC=ZETAE-GAMAE                                                   TDETA
      V(II)=BETAE+2.*ZETAE                                              TDETA
      W(II)=0.                                                          TDETA
      GO TO 230
  220 CIP1J=C(II+2,J)                                                   TDETA
      AFC=ZETAE                                                         TDETA
      V(II)=BETAE                                                       TDETA
      W(II)=-GAMAE*CSTAR(II+2,J)                                        TDETA
  230 CIJ=C(II,J)                                                       TDETA
      CIM1J=C(II-1,J)                                                   TDETA
      CIJM1=SIGM*C(II,JM1)+SM*C(II,1)                                   TDETA
      CIJP1=SIGP*C(II,JP1)+SP*C(II,JJ)                                  TDETA
      W(II)=W(II)+SUMF(DELTA1,CIM1J,DELTA2,CIJ,DELTA3,CIP1J,            TDETA
     1DELTA4,CIJM1,DELTA5,CIJP1)                                        TDETA
      W(II)=W(II)-W(II-1)*AFC/V(II-1)                                   TDETA
      V(II)=V(II)-(GFC*AFC)/V(II-1)                                     TDETA
      CSTAR(II,J)=W(II)/V(II)                                           TDETA
      IIM2=II-2                                                         TDETA
      DO 240 I=1,IIM2                                                   TDETA
      IREV=II-I                                                         TDETA
      CALL C4ETA(IREV,J)                                                TDETA
  240 CSTAR(IREV,J)=(W(IREV)-GAMAE*CSTAR(IREV+1,J))/V(IREV)             TDETA
      I=1                                                               TDETA
      CALL C4ETA (1,J)                                                  TDETA
      GO TO (250,260,270),KFETA                                         TDETA
  250 GFC=GAMAE+ZETAE                                                   TDETA
      GO TO 280                                                         TDETA
  260 GFC=GAMAE-ZETAE                                                   TDETA
      GO TO 280                                                         TDETA
  270 GFC=GAMAE                                                         TDETA
  280 CSTAR(1,J)=(W(1)-GFC*CSTAR(2,J))/V(1)                             TDETA
 2000 CONTINUE                                                          TDETA
      RETURN                                                            TDETA
      END                                                               TDETA
                                                                        TDETA


      SUBROUTINE C4ETA(I,J)
*     SYMBOL TABLE                                                      C4ETA1
*     LABEL                                                             C4ETA1
C     C4ETA(I,J) GIVES THE COEFFICIENTS FOR THE ETA-EQUATION            C4ETA1
C     AT THE POINT (I,J).                                               C4ETA1
C     C4ETA1 IS FOR ONE DIMENSIONAL FLOW IN HOMOGENEOUS MEDIA.          C4ETA1
      DIMENSION C(53,53),CSTAR(53,53),CSS(53,53)                        C4ETA1
      COMMON C,CSTAR,CSS,II,JJ,DTIME,DETA,DCSI,ALFALP,ALFATP,DMOLP,     C4ETA1
     1UZERO,ELZERO,ETAMIN,CSIMIN,EPSAB,A1,A2,A3,A4,B1,B2,B3,            C4ETA1
     2KFETA,CFETA,KLETA,CLETA,KFCSI,CFCSI,KLCSI,CLCSI,                  C4ETA1
     3ZETAE,BETAE,GAMAE,DELTA1,DELTA2,DELTA3,DELTA4,DELTA5,             C4ETA1
     4ZETAC,BETAC,GAMAC,DELTA6,DELTA7,DELTA8,DELTA9,DELT10,RO1,RO2,RO3  C4ETA1
      DESQ=DETA*DETA                                                    C4ETA1
      DCSQ=DCSI*DCSI                                                    C4ETA1
      ETA=ETAMIN+DETA*FLOATF(I-1)                                       C4ETA1
      CSI=CSIMIN+DCSI*FLOATF(J-1)                                       C4ETA1
      VIJ=1.0                                                           C4ETA1
      VIP1J=VIJ                                                         C4ETA1
      VIM1J=VIJ                                                         C4ETA1
                                                                        C4ETA1
      VIJP1=VIJ                                                         C4ETA1
      VIJM1=VIJ                                                         C4ETA1
      DLP=0.5*ALFALP*(VIP1J+VIJ)+DMOLP                                  C4ETA1
      DLM=0.5*ALFALP*(VIJ+VIM1J)+DMOLP                                  C4ETA1
      DTP=0.5*ALFATP*(VIJP1+VIJ)+DMOLP                                  C4ETA1
      DTM=0.5*ALFATP*(VIJ+VIJM1)+DMOLP                                  C4ETA1
      VDT=VIJ*VIJ*DTIME                                                 C4ETA1
      ZETAE=B3/VDT-DLM/DESQ-A4/DETA                                     C4ETA1
      BETAE=B1/VDT+(DLP+DLM)/DESQ+(A4-A3)/DETA                          C4ETA1
      GAMAE=B2/VDT-DLP/DESQ+A3/DETA                                     C4ETA1
      DELTA1=B3/VDT+A2/DETA                                             C4ETA1
      DELTA2=B1/VDT-(DTM+DTP)/DCSQ+(A1-A2)/DETA                         C4ETA1
      DELTA3=B2/VDT-A1/DETA                                             C4ETA1
      DELTA4=DTM/DCSQ                                                   C4ETA1
   10 DELTA5=DTP/DCSQ                                                   C4ETA1
      RETURN                                                            C4ETA1
      END                                                               C4ETA1


      SUBROUTINE TDCSI
*     SYMBOL TABLE                                                      TDCSI
*     LABEL                                                             TDCSI
C     TDCSI SOLVES THE TRI-DIAGONAL MATRIX OF THE CSI-EQUATION          TDCSI
C     FOR CSS USING C AND CSTAR.                                        TDCSI
      DIMENSION C(53,53),CSTAR(53,53),CSS(53,53),V(53),W(53)            TDCSI
      COMMON C,CSTAR,CSS,II,JJ,DTIME,DETA,DCSI,ALFALP,ALFATP,DMOLP,     TDCSI
     1UZERO,ELZERO,ETAMIN,CSIMIN,EPSAB,A1,A2,A3,A4,B1,B2,B3,            TDCSI
     2KFETA,CFETA,KLETA,CLETA,KFCSI,CFCSI,KLCSI,CLCSI,                  TDCSI
     3ZETAE,BETAE,GAMAE,DELTA1,DELTA2,DELTA3,DELTA4,DELTA5,             TDCSI
     4ZETAC,BETAC,GAMAC,DELTA6,DELTA7,DELTA8,DELTA9,DELT10,RO1,RO2,RO3  TDCSI
      SUMF(S1,P1,S2,P2,S3,P3,S4,P4,S5,P5)=S1*P1+S2*P2+S3*P3+S4*P4+S5*P5 TDCSI
      DO 550 I=1,II                                                     TDCSI
      IF (I-1) 300,300,310                                              TDCSI
  300 IM1=2                                                             TDCSI
      GO TO (320,330,340),KFETA                                         TDCSI
  320 SIGM=1.                                                           TDCSI
      SM=0.                                                             TDCSI
      GO TO 370                                                         TDCSI
  330 SIGM=-1.                                                          TDCSI
      SM=2.                                                             TDCSI
      GO TO 370                                                         TDCSI
  340 SIGM=1.                                                           TDCSI
      SM=0.                                                             TDCSI
      IM1=II+1                                                          TDCSI
      GO TO 370                                                         TDCSI
  310 IM1=I-1                                                           TDCSI
      SIGM=1.                                                           TDCSI
      SM=0.                                                             TDCSI
      IF (II-I) 360,360,370                                             TDCSI
  360 IP1=II-1                                                          TDCSI
      GO TO (380,390,400),KLETA                                         TDCSI
  380 SIGP=1.                                                           TDCSI
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      SP=0.                                                             TDCSI
      GO TO 410                                                         TDCSI
 390  SIGP=-1.                                                          TDCSI
      SP=2.                                                             TDCSI
      GO TO 410                                                         T4359
 400  SIGP=1.                                                           TDCSI
      SP=0.                                                             TDCSI
      IP1=II+2                                                          TDCSI
      GO TO 410                                                         TDCSI
 370  IP1=I+1                                                           TDCSI
      SIGP=1.                                                           TDCSI
      SP=0.                                                             TDCSI
 410  CIJ=C(I,1)                                                        TDCSI
      CIJP1=C(I,2)                                                      TDCSI
      CALL C4CSI (I,1)                                                  TDCSI
      GO TO (420,430,440),KFCSI                                         TDCSI
 420  CIJM1=C(I,2)                                                      TDCSI
      GFC=GAMAC+ZETAC                                                   TDCSI
      V(1)=BETAC                                                        TDCSI
      W(1)=0.                                                           TDCSI
      GO TO 450                                                         TDCSI
 430  CIJM1=-C(I,2)+2.*C(I,1)                                           TDCSI
      GFC=GAMAC-ZETAC                                                   TDCSI
      V(1)=BETAC+2.*ZETAC                                               TDCSI
      W(1)=0.                                                           TDCSI
      GO TO 450                                                         TDCSI
 440  CIJM1=C(I,JJ+1)                                                   TDCSI
      GFC=GAMAC                                                         TDCSI
      V(1)=BETAC                                                        TDCSI
      W(1)=-ZETAC*C(I,JJ+1)                                             TDCSI
 450  CIM1J=SIGM*C(IM1,1)+SM*C(1,1)                                     TDCSI
      CIP1J=SIGP*C(IP1,1)+SP*C(II,1)                                    TDCSI
      W(1)=W(1)+SUMF(DELTA6,CIJM1,DELTA7,CIJ,DELTA8,CIJP1,              TDCSI
     1DELTA9,CIM1J,DELT10,CIP1J)                                        TDCSI
      CSI=CSTAR(I,1)                                                    TDCSI
      CSIM1=SIGM*CSTAR(IM1,1)+SM*CSTAR(1,1)                             TDCSI
      CSIP1=SIGP*CSTAR(IP1,1)+SP*CSTAR(II,1)                            TDCSI
      W(1)=W(1)+RO1*CSI+RO2*CSIP1+RO3*CSIM1                             TDCSI
      JJM1=JJ-1                                                         TDCSI
      DO 460 J=2,JJM1                                                   TDCSI
      CALL C4CSI (I,J)                                                  TDCSI
      V(J)=BETAC-(GFC*ZETAC)/V(J-1)                                     TDCSI
      CIJ=C(I,J)                                                        TDCSI
      CIJM1=C(I,J-1)                                                    TDCSI
      CIJP1=C(I,J+1)                                                    TDCSI
      CIM1J=SIGM*C(IM1,J)+SM*C(1,J)                                     TDCSI
      CIP1J=SIGP*C(IP1,J)+SP*C(II,J)                                    TDCSI
      RHS=SUMF(DELTA6,CIJM1,DELTA7,CIJ,DELTA8,CIJP1,DELTA9,CIM1J,       TDCSI
     1DELT10,CIP1J)                                                     TDCSI
      CSI=CSTAR(I,J)                                                    TDCSI
      CSIM1=SIGM*CSTAR(IM1,J)+SM*CSTAR(1,J)                             TDCSI
      CSIP1=SIGP*CSTAR(IP1,J)+SP*CSTAR(II,J)                            TDCSI
      RHS=RHS+RO1*CSI+RO2*CSIP1+RO3*CSIM1                               TDCSI
      W(J)=RHS-(W(J-1)*ZETAC)/V(J-1)                                    TDCSI
 460  GFC=GAMAC                                                         TDCSI
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```
      J=JJ
      CALL C4CSI (I,JJ)                                                 TDCSI
      GO TO (470,480,490),KLCSI                                         TDCSI
  470 CIJP1=C(I,JJ-1)                                                   TDCSI
      AFC=ZETAC+GAMAC                                                   TDCSI
      V(JJ)=BETAC                                                       TDCSI
      W(JJ)=0.                                                          TDCSI
      GO TO 500                                                         TDCSI
  480 CIJP1=-C(I,JJ-1)+2.*C(I,JJ)                                       TDCSI
      AFC=ZETAC-GAMAC                                                   TDCSI
      V(JJ)=BETAC+2.*ZETAC                                              TDCSI
      W(JJ)=0.                                                          TDCSI
      GO TO 500                                                         TDCSI
  490 CIJP1=C(I,JJ+2)                                                   TDCSI
      AFC=ZETAC                                                         TDCSI
      V(JJ)=BETAC                                                       TDCSI
      W(JJ)=-GAMAC*C(I,JJ+2)                                            TDCSI
  500 CIJ=C(I,JJ)                                                       TDCSI
      CIJM1=C(I,JJ-1)                                                   TDCSI
      CIM1J=SIGM*C(IM1,JJ)+SM*C(1,JJ)                                   TDCSI
      CIP1J=SIGP*C(IP1,JJ)+SP*C(II,JJ)                                  TDCSI
      W(JJ)=W(JJ)+SUMF(DELTA6,CIJM1,DELTA7,CIJ,DELTA8,CIJP1,            TDCSI
     1DELTA9,CIM1J,DELT10,CIP1J)                                        TDCSI
      CSI=CSTAR(I,JJ)                                                   TDCSI
      CSIM1=SIGM*CSTAR(IM1,JJ)+SM*CSTAR(1,JJ)                           TDCSI
      CSIP1=SIGP*CSTAR(IP1,JJ)+SP*CSTAR(II,JJ)                          TDCSI
      W(JJ)=W(JJ)+RO1*CSI+RO2*CSIP1+RO3*CSIM1                           TDCSI
      W(JJ)=W(JJ)-W(JJ-1)*AFC/V(JJ-1)                                   TDCSI
      V(JJ)=V(JJ)-(GFC*AFC)/V(JJ-1)                                     TDCSI
      CSS(I,JJ)=W(JJ)/V(JJ)                                             TDCSI
      JJM2=JJ-2                                                         TDCSI
      DO 510 J=1,JJM2                                                   TDCSI
      JREV=JJ-J                                                         TDCSI
      CALL C4CSI(I,JREV)                                                TDCSI
  510 CSS(I,JREV)=(W(JREV)-GAMAC*CSS(I,JREV+1))/V(JREV)                 TDCSI
      J=1                                                               TDCSI
      CALL C4CSI (I,1)                                                  TDCSI
      GO TO (520,530,540),KFCSI                                         TDCSI
  520 GFC=GAMAC+ZETAC                                                   TDCSI
      GO TO 550                                                         TDCSI
  530 GFC=GAMAC-ZETAC                                                   TDCSI
      GO TO 550                                                         TDCSI
  540 GFC=GAMAC                                                         TDCSI
  550 CSS(I,1)=(W(1)-GFC*CSS(I,2))/V(1)                                 TDCSI
 2000 CONTINUE                                                          TDCSI
      RETURN                                                            TDCSI
      END                                                               TDCSI
                                                                        TDCSI



      SUBROUTINE C4CSI(I,J)
*     SYMBOL TABLE                                                      C4CSI1
*     LABEL                                                             C4CSI1
                                                                        C4CSI1
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*     LIST 8
C     C4CSI(I,J) GIVES THE COEFFICIENTS FOR THE CSI-EQUATION            C4CSI1
C     AT THE POINT (I,J).                                               C4CSI1
C     C4CSI1 IS FOR ONE DIMENSIONAL FLOW IN HOMOGENEOUS MEDIA.          C4CSI1
      DIMENSION C(53,53),CSTAR(53,53),CSS(53,53)                        C4CSI1
      COMMON C,CSTAR,CSS,II,JJ,DTIME,DETA,DCSI,ALFALP,ALFATP,DMOLP,     C4CSI1
     1UZERO,ELZERO,ETAMIN,CSIMIN,EPSAB,A1,A2,A3,A4,B1,B2,B3,            C4CSI1
     2KFETA,CFETA,KLETA,CLETA,KFCSI,CFCSI,KLCSI,CLCSI,                  C4CSI1
     3ZETAE,BETAE,GAMAE,DELTA1,DELTA2,DELTA3,DELTA4,DELTA5,             C4CSI1
     4ZETAC,BETAC,GAMAC,DELTA6,DELTA7,DELTA8,DELTA9,DELT10,RO1,RO2,RO3  C4CSI1
      DESQ=DETA*DETA                                                    C4CSI1
      DCSQ=DCSI*DCSI                                                    C4CSI1
      ETA=ETAMIN+DETA*FLOATF(I-1)                                       C4CSI1
      CSI=CSIMIN+DCSI*FLOATF(J-1)                                       C4CSI1
      VIJ=1.0                                                           C4CSI1
      VIJP1=VIJ                                                         C4CSI1
      VIJM1=VIJ                                                         C4CSI1
      DTP=0.5*ALFATP*(VIJP1+VIJ)+DMOLP                                  C4CSI1
      DTM=0.5*ALFATP*(VIJ+VIJM1)+DMOLP                                  C4CSI1
      VDT=VIJ*VIJ*DTIME                                                 C4CSI1
      ZETAC=-DTM/DCSQ                                                   C4CSI1
      BETAC=B1/VDT+(DTM+DTP)/DCSQ                                       C4CSI1
      GAMAC=-DTP/DCSQ                                                   C4CSI1
      DELTA6=ZETAC                                                      C4CSI1
      DELTA7=(DTM+DTP)/DCSQ                                             C4CSI1
      DELTA8=GAMAC                                                      C4CSI1
      DELTA9=0.                                                         C4CSI1
      DELT10=0.                                                         C4CSI1
      RO1=B1/VDT                                                        C4CSI1
      RO2=0.                                                            C4CSI1
   10 RO3=0.                                                            C4CSI1
      RETURN                                                            C4CSI1
      END                                                               C4CSI1
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      SUBROUTINE EXPLIC                                                 EXPLIC
*     SYMBOL TABLE                                                      EXPLIC
*     LABEL                                                             EXPLIC
C     EXPLIC SOLVES EXPLICITELY FOR C(N+1) USING C, CSTAR AND CSS.      EXPLIC
C     THE SOLUTION PROCEEDS A WHOLE ROW AT A TIME, RESULTS ARE STORED   EXPLIC
C     IN CTEMP(I) AND THEN PUT IN C (WHICH IS NOT NEEDED ANY MORE).     EXPLIC
      DIMENSION C(53,53),CSTAR(53,53),CSS(53,53),CTEMP(53)              EXPLIC
      COMMON C,CSTAR,CSS,II,JJ,DTIME,DETA,DCSI,ALFALP,ALFATP,DMOLP,     EXPLIC
     1UZERO,ELZERO,ETAMIN,CSIMIN,EPSAB,A1,A2,A3,A4,B1,B2,B3,            EXPLIC
     2KFETA,CFETA,KLETA,CLETA,KFCSI,CFCSI,KLCSI,CLCSI,                  EXPLIC
     3ZETAE,BETAE,GAMAE,DELTA1,DELTA2,DELTA3,DELTA4,DELTA5,             EXPLIC
     4ZETAC,BETAC,GAMAC,DELTA6,DELTA7,DELTA8,DELTA9,DELT10,RO1,RO2,RO3, EXPLIC
     5P1,P2,P3,Q1,Q2,Q3,S1,S2,S3                                        EXPLIC
      DO 220 J=1,JJ                                                     EXPLIC
      IF (J-1) 10,10,50                                                 EXPLIC
   10 GO TO (20,30,40),KFCSI                                            EXPLIC
   20 JM1=2                                                             EXPLIC
```

```
      SIGM=1.                                                           EXPLIC
      SM=0.                                                             EXPLIC
      GO TO 100                                                         EXPLIC
   30 JM1=2                                                             EXPLIC
      SIGM=-1.                                                          EXPLIC
      SM=2.                                                             EXPLIC
      GO TO 100                                                         EXPLIC
   40 JM1=JJ+1                                                          EXPLIC
      SIGM=1.                                                           EXPLIC
      SM=0.                                                             EXPLIC
      GO TO 100                                                         EXPLIC
   50 JM1=J-1                                                           EXPLIC
      SIGM=1.                                                           EXPLIC
      SM=0.                                                             EXPLIC
      IF (JJ-J) 60,60,100                                               EXPLIC
   60 GO TO (70,80,90),KLCSI                                            EXPLIC
   70 JP1=JJ-1                                                          EXPLIC
      SIGP=1.                                                           EXPLIC
      SP=0.                                                             EXPLIC
      GO TO 110                                                         EXPLIC
   80 JP1=JJ-1                                                          EXPLIC
      SIGP=-1.                                                          EXPLIC
      SP=2.                                                             EXPLIC
      GO TO 110                                                         EXPLIC
   90 JP1=JJ+2                                                          EXPLIC
      SIGP=1.                                                           EXPLIC
      SP=0.                                                             EXPLIC
      GO TO 110                                                         EXPLIC
  100 JP1=J+1                                                           EXPLIC
      SIGP=1.                                                           EXPLIC
      SP=0.                                                             EXPLIC
  110 CALL CFEXP (1,J)                                                  EXPLIC
      GO TO (120,130,140),KFETA                                         EXPLIC
  120 CTEMP(1)=P2*C(2,J)+Q1*CSTAR(2,J)                                  EXPLIC
      GO TO 150                                                         EXPLIC
  130 CTEMP(1)=P2*(2.*C(1,J)-C(2,J))+Q1*(2.*CSTAR(1,J)-CSTAR(2,J))      EXPLIC
      GO TO 150                                                         EXPLIC
  140 CTEMP(1)=P2*C(II+1,J)+Q1*CSTAR(II+1,J)                            EXPLIC
  150 CTEMP(1)=CTEMP(1)+P1*C(1,J)+P3*C(2,J)+Q2*CSTAR(1,J)+Q3*CSTAR(2,J) EXPLIC
     1+S1*(SIGM*CSS(1,JM1)+SM*CSS(1,1))+S2*CSS(1,J)+S3*(SIGP*CSS(1,JP1) EXPLIC
     1+SP*CSS(1,JJ))                                                    EXPLIC
      IIM1=II-1                                                         EXPLIC
      DO 160 I=2,IIM1                                                   EXPLIC
      CALL CFEXP (I,J)                                                  EXPLIC
      CTEMP(I)=P1*C(I,J)+P2*C(I-1,J)+P3*C(I+1,J)+Q1*CSTAR(I-1,J)+       EXPLIC
     1Q2*CSTAR(I,J)+Q3*CSTAR(I+1,J)+S1*(SIGM*CSS(I,JM1)+SM*CSS(I,1))+   EXPLIC
     1S2*CSS(I,J)+S3*(SIGP*CSS(I,JP1)+SP*CSS(I,JJ))                     EXPLIC
  160 CONTINUE                                                          EXPLIC
      I=II                                                              EXPLIC
      CALL CFEXP (II,J)                                                 EXPLIC
      GO TO (170,180,190),KLETA                                         EXPLIC
  170 CTEMP(II)=P3*C(II-1,J)+Q3*CSTAR(II-1,J)                           EXPLIC
      GO TO 200                                                         EXPLIC
  180 CTEMP(II)=P3*(2.*C(II,J)-C(II-1,J))+Q3*(2.*CSTAR(II,J)-           EXPLIC
     1CSTAR(II-1,J))                                                    EXPLIC
```

```
      GO TO 200                                                         EXPLIC
  190 CTEMP(II)=P3*C(II+2,J)+Q3*CSTAR(II+2,J)                           EXPLIC
  200 CTEMP(II)=CTEMP(II)+P1*C(II,J)+P2*C(II-1,J)+                      EXPLIC
     1Q1*CSTAR(II-1,J)+Q2*CSTAR(II,J)+S1*(SIGM*CSS(II,JM1)+             EXPLIC
     1SM*CSS(II,1))+S2*CSS(II,J)+S3*(SIGP*CSS(II,JP1)+SP*CSS(II,JJ))    EXPLIC
      DO 210 I=1,II                                                     EXPLIC
  210 C(I,J)=CTEMP(I)                                                   EXPLIC
  220 CONTINUE                                                          EXPLIC
      RETURN                                                            EXPLIC
      END                                                               EXPLIC
```

```
      SUBROUTINE CFEXP (I,J)                                            CFEXP1
*     SYMBOL TABLE                                                      CFEXP1
*     LABEL                                                             CFEXP1
*     LIST 8                                                            CFEXP1
C     CFEXP(I,J) GIVES THE COEFFICIENTS FOR THE EXPLICIT EQUATION       CFEXP1
C     AT THE POINT (I,J).                                               CFEXP1
C     CFEXP1 IS FOR ONE DIMENSIONAL FLOW IN HOMOGENEOUS MEDIA.          CFEXP1
      DIMENSION C(53,53),CSTAR(53,53),CSS(53,53)                        CFEXP1
      COMMON C,CSTAR,CSS,II,JJ,DTIME,DETA,DCSI,ALFALP,ALFATP,DMOLP,     CFEXP1
     1UZERO,ELZERO,ETAMIN,CSIMIN,EPSAB,A1,A2,A3,A4,B1,B2,B3,            CFEXP1
     2KFETA,CFETA,KLETA,CLETA,KFCSI,CFCSI,KLCSI,CLCSI,                  CFEXP1
     3ZETAE,BETAE,GAMAE,DELTA1,DELTA2,DELTA3,DELTA4,DELTA5,             CFEXP1
     4ZETAC,BETAC,GAMAC,DELTA6,DELTA7,DELTA8,DELTA9,DELT10,RO1,RO2,RO3, CFEXP1
     5P1,P2,P3,Q1,Q2,Q3,S1,S2,S3                                        CFEXP1
      DESQ=DETA*DETA                                                    CFEXP1
      DCSQ=DCSI*DCSI                                                    CFEXP1
      ETA=ETAMIN+DETA*FLOATF(I-1)                                       CFEXP1
      CSI=CSIMIN+DCSI*FLOATF(J-1)                                       CFEXP1
      VIJ=1.0                                                           CFEXP1
      VIP1J=VIJ                                                         CFEXP1
      VIM1J=VIJ                                                         CFEXP1
      VIJP1=VIJ                                                         CFEXP1
      VIJM1=VIJ                                                         CFEXP1
      DLP=0.5*ALFALP*(VIP1J+VIJ)+DMOLP                                  CFEXP1
      DLM=0.5*ALFALP*(VIJ+VIM1J)+DMOLP                                  CFEXP1
      DTP=0.5*ALFATP*(VIJP1+VIJ)+DMOLP                                  CFEXP1
      DTM=0.5*ALFATP*(VIJ+VIJM1)+DMOLP                                  CFEXP1
      VDT=VIJ*VIJ*DTIME                                                 CFEXP1
      P1=1.+(A1-A2)*VDT/DETA                                            CFEXP1
      P2=A2*VDT/DETA                                                    CFEXP1
      P3=-A1*VDT/DETA                                                   CFEXP1
      Q1=DLM*VDT/DESQ+A4*VDT/DETA                                       CFEXP1
      Q2=-(DLM+DLP)*VDT/DESQ+(A3-A4)*VDT/DETA                           CFEXP1
      Q3=DLP*VDT/DESQ-A3*VDT/DETA                                       CFEXP1
      S1=DTM*VDT/DCSQ                                                   CFEXP1
      S2=-(DTM+DTP)*VDT/DCSQ                                            CFEXP1
   10 S3=DTP*VDT/DCSQ                                                   CFEXP1
      RETURN                                                            CFEXP1
      END                                                               CFEXP1
      SUBROUTINE CINPUT (CSINN,CSINX,KIN)                               CINPUT
*     SYMBOL TABLE                                                      CINPUT
*     LABEL                                                             CINPUT
C     CINPUT GIVES THE INPUT CONCENTRATION AT ETA=ETAMIN,               CINPUT
C     BETWEEN CSI=CSINN AND CSI=CSINX, AND STORES IT IN C(II+1,J).      CINPUT
C     KIN=1 C(ETAMIN,CSI)=CFETA OVER CSINN TO CSINX                     CINPUT
C     KIN=2 SAME AS KIN=1 EXCEPT C(ETAMIN,CSINX)=CFETA/2.               CINPUT
      DIMENSION C(53,53),CSTAR(53,53),CSS(53,53)                        CINPUT
      COMMON C,CSTAR,CSS,II,JJ,DTIME,DETA,DCSI,ALFALP,ALFATP,DMOLP,      CINPUT
     1UZERO,ELZERO,ETAMIN,CSIMIN,EPSAB,A1,A2,A3,A4,B1,B2,B3,            CINPUT
     2KFETA,CFETA,KLETA,CLETA,KFCSI,CFCSI,KLCSI,CLCSI,                  CINPUT
     3ZETAE,BETAE,GAMAE,DELTA1,DELTA2,DELTA3,DELTA4,DELTA5,             CINPUT
     4ZETAC,BETAC,GAMAC,DELTA6,DELTA7,DELTA8,DELTA9,DELT10,RO1,RO2,RO3  CINPUT
      JMAX=CSINX/DCSI+1.                                                CINPUT
      JMIN=CSINN/DCSI+1.                                                CINPUT
      GO TO (10,30,50),KIN                                              CINPUT
   10 DO 20 J=JMIN,JMAX                                                 CINPUT
      C(II+1,J)=CFETA                                                   CINPUT
      CSTAR(II+1,J)=CFETA                                               CINPUT
   20 CSS(II+1,J)=CFETA                                                 CINPUT
      GO TO 60                                                          CINPUT
   30 C(II+1,JMAX)=CFETA/2.                                             CINPUT
      CSTAR(II+1,JMAX)=CFETA/2.                                         CINPUT
      CSS(II+1,JMAX)=CFETA/2.                                           CINPUT
      J2=JMAX-1                                                         CINPUT
      DO 40 J=JMIN,J2                                                   CINPUT
      C(II+1,J)=CFETA                                                   CINPUT
      CSTAR(II+1,J)=CFETA                                               CINPUT
   40 CSS(II+1,J)=CFETA                                                 CINPUT
      GO TO 60                                                          CINPUT
C     50 IS A DUMMY STATEMENT FOR ADDING MORE TYPES OF INPUT.           CINPUT
   50 CONTINUE                                                          CINPUT
   60 RETURN                                                            CINPUT
      END                                                               CINPUT


      SUBROUTINE USPRNT (T,IPRNT,ISTEP,JSTEP)                           USPRNT
*     SYMBOL TABLE                                                      USPRNT
*     LABEL                                                             USPRNT
C     IPRNT=1 PRINT OUT THE WHOLE ARRAY.                                USPRNT
C     IPRNT=2 PRINT OUT ONLY EVERY ISTEP IN ETA AND JSTEP IN CSI.       USPRNT
      DIMENSION C(53,53),CSTAR(53,53),CSS(53,53),JP(53)                 USPRNT
      COMMON C,CSTAR,CSS,II,JJ,DTIME,DETA,DCSI,ALFALP,ALFATP,DMOLP,      USPRNT
     1UZERO,ELZERO,ETAMIN,CSIMIN,EPSAB,A1,A2,A3,A4,B1,B2,B3,            USPRNT
     2KFETA,CFETA,KLETA,CLETA,KFCSI,CFCSI,KLCSI,CLCSI,                  USPRNT
     3ZETAE,BETAE,GAMAE,DELTA1,DELTA2,DELTA3,DELTA4,DELTA5,             USPRNT
     4ZETAC,BETAC,GAMAC,DELTA6,DELTA7,DELTA8,DELTA9,DELT10,RO1,RO2,RO3  USPRNT
      PRINT 1000,T                                                      USPRNT
 1000 FORMAT(//21H RELATIVE CONC. AT T=F15.5//)                         USPRNT
      NN=II/10                                                          USPRNT
      IF (10*NN-II) 1,2,2                                               USPRNT
    1 NN=NN+1                                                           USPRNT
    2 GO TO (10,70),IPRNT                                               USPRNT
   10 DO 50 J=1,JJ                                                      USPRNT
      CSI=CSIMIN+DCSI*FLOATF(J-1)                                       USPRNT
      PRINT 1001,J,CSI                                                  USPRNT
 1001 FORMAT (5H C(I,I3,8H)=C(ETA,,F10.5,1H),)                          USPRNT
      DO 50 N=1,NN                                                      USPRNT
      IBEG=10*N-9                                                       USPRNT
      IF (C(IBEG,J)-0.01) 50,20,20                                      USPRNT
   20 IEND=10*N                                                         USPRNT
      IF (II-IEND) 30,40,40                                             USPRNT
   30 IEND=II                                                           USPRNT
   40 PRINT 1004,IBEG,IEND,(C(I,J),I=IBEG,IEND)                         USPRNT
 1004 FORMAT(3H I=I3,6H TO I=I3,10F10.5)                                USPRNT
   50 CONTINUE                                                          USPRNT
      GO TO 120                                                         USPRNT
   70 DO 80 J=1,JJ,JSTEP                                                USPRNT
   80 JP(J)=J                                                           USPRNT
      PRINT 1002,(JP(J),J=1,JJ,JSTEP)                                   USPRNT
 1002 FORMAT (1H ,13(7X,I3))                                            USPRNT
      DO 100 I=1,II,ISTEP                                               USPRNT
      SUM=0.                                                            USPRNT
      DO 90 J=1,JJ                                                      USPRNT
   90 SUM=SUM+C(I,J)                                                    USPRNT
      IF (SUM-0.1) 110,110,100                                          USPRNT
  100 PRINT 1003,I,(C(I,J),J=1,JJ,JSTEP)                                USPRNT
 1003 FORMAT (1H I3,13F10.5)                                            USPRNT
  110 CONTINUE                                                          USPRNT
  120 RETURN                                                            USPRNT
      END                                                               USPRNT
```

```
      SUBROUTINE USMAP(T)                                               USMAP
*     SYMBOL TABLE                                                      USMAP
*     LABEL                                                             USMAP
*     LIST 8                                                            USMAP
      DIMENSION C(53,53),CSTAR(53,53),CSS(53,53),DENS(46,3),P(55,3)     USMAP
      COMMON C,CSTAR,CSS,II,JJ,DTAU,DETA,DCSI,ALFALP,ALFATP,DMOLP,      USMAP
     1UZERO,ELZERO,ETAMIN,CSIMIN,EPSAB,A1,A2,A3,A4,B1,B2,B3,            USMAP
     2KFETA,CFETA,KLETA,CLETA,KFCSI,CFCSI,KLCSI,CLCSI,                  USMAP
     3ZETAE,BETAE,GAMAE,DELTA1,DELTA2,DELTA3,DELTA4,DELTA5,             USMAP
     4ZETAC,BETAC,GAMAC,DELTA6,DELTA7,DELTA8,DELTA9,DELT10,RO1,RO2,RO3, USMAP
     5ITABLE                                                            USMAP
      PRINT 500,T                                                       USMAP
  500 FORMAT (1H1,6H TIME=F10.5)                                        USMAP
      IF (ITABLE-15) 10,20,10                                           USMAP
   10 DENS( 1,1)=1H                                                     USMAP
      DENS( 1,2)=1H                                                     USMAP
      DENS( 1,3)=1H                                                     USMAP
      DENS( 2,1)=1H                                                     USMAP
      DENS( 2,2)=1H                                                     USMAP
      DENS( 2,3)=1H.                                                    USMAP
      DENS( 3,1)=1H                                                     USMAP
      DENS( 3,2)=1H                                                     USMAP
      DENS( 3,3)=1H,                                                    USMAP
      DENS( 4,1)=1H                                                     USMAP
      DENS( 4,2)=1H,                                                    USMAP
      DENS( 4,3)=1H.                                                    USMAP
      DENS( 5,1)=1H                                                     USMAP
      DENS( 5,2)=1H-                                                    USMAP
      DENS( 5,3)=1H.                                                    USMAP
      DENS( 6,1)=1H                                                     USMAP
      DENS( 6,2)=1H-                                                    USMAP
      DENS( 6,3)=1H,                                                    USMAP
      DENS( 7,1)=1H                                                     USMAP
      DENS( 7,2)=1H,                                                    USMAP
      DENS( 7,3)=1H-                                                    USMAP
      DENS( 8,1)=1H=                                                    USMAP
      DENS( 8,2)=1H                                                     USMAP
      DENS( 8,3)=1H=                                                    USMAP
      DENS( 9,1)=1H                                                     USMAP
      DENS( 9,2)=1H+                                                    USMAP
      DENS( 9,3)=1H+                                                    USMAP
      DENS(10,1)=1H+                                                    USMAP
      DENS(10,2)=1H-                                                    USMAP
      DENS(10,3)=1H+                                                    USMAP
      DENS(11,1)=1H=                                                    USMAP
      DENS(11,2)=1H,                                                    USMAP
      DENS(11,3)=1H=                                                    USMAP
      DENS(12,1)=1H                                                     USMAP
      DENS(12,2)=1H,                                                    USMAP
      DENS(12,3)=1H/                                                    USMAP
      DENS(13,1)=1H                                                     USMAP
      DENS(13,2)=1H-                                                    USMAP
      DENS(13,3)=1H/                                                    USMAP
      DENS(14,1)=1H                                                     USMAP
      DENS(14,2)=1H,                                                    USMAP
      DENS(14,3)=1H+                                                    USMAP
      DENS(15,1)=1H                                                     USMAP
      DENS(15,2)=1HX                                                    USMAP
      DENS(15,3)=1HX                                                    USMAP
      DENS(16,1)=1HL                                                    USMAP
      DENS(16,2)=1HL                                                    USMAP
      DENS(16,3)=1H,                                                    USMAP
      DENS(17,1)=1HL                                                    USMAP
      DENS(17,2)=1HL                                                    USMAP
      DENS(17,3)=1H-                                                    USMAP
      DENS(18,1)=1H=                                                    USMAP
      DENS(18,2)=1HY                                                    USMAP
      DENS(18,3)=1H=                                                    USMAP
      DENS(19,1)=1H                                                     USMAP
      DENS(19,2)=1HL                                                    USMAP
      DENS(19,3)=1H=                                                    USMAP
      DENS(20,1)=1H-                                                    USMAP
      DENS(20,2)=1HY                                                    USMAP
      DENS(20,3)=1H,                                                    USMAP
      DENS(21,1)=1H+                                                    USMAP
      DENS(21,2)=1HL                                                    USMAP
      DENS(21,3)=1H+                                                    USMAP
      DENS(22,1)=1HL                                                    USMAP
      DENS(22,2)=1H,                                                    USMAP
      DENS(22,3)=1H=                                                    USMAP
      DENS(23,1)=1H                                                     USMAP
      DENS(23,2)=1HO                                                    USMAP
      DENS(23,3)=1H-                                                    USMAP
      DENS(24,1)=1H=                                                    USMAP
      DENS(24,2)=1HL                                                    USMAP
      DENS(24,3)=1H/                                                    USMAP
      DENS(25,1)=1HL                                                    USMAP
      DENS(25,2)=1H/                                                    USMAP
      DENS(25,3)=1HY                                                    USMAP
      DENS(26,1)=1H                                                     USMAP
      DENS(26,2)=1HO                                                    USMAP
      DENS(26,3)=1H=                                                    USMAP
      DENS(27,1)=1H=                                                    USMAP
      DENS(27,2)=1H+                                                    USMAP
      DENS(27,3)=1HX                                                    USMAP
      DENS(28,1)=1HO                                                    USMAP
      DENS(28,2)=1H,                                                    USMAP
      DENS(28,3)=1H=                                                    USMAP
      DENS(29,1)=1HT                                                    USMAP
      DENS(29,2)=1H=                                                    USMAP
      DENS(29,3)=1HX                                                    USMAP
      DENS(30,1)=1HU                                                    USMAP
      DENS(30,2)=1H=                                                    USMAP
      DENS(30,3)=1HY                                                    USMAP
      DENS(31,1)=1HT                                                    USMAP
      DENS(31,2)=1H-                                                    USMAP
      DENS(31,3)=1HU                                                    USMAP
      DENS(32,1)=1H                                                     USMAP
      DENS(32,2)=1HU                                                    USMAP
      DENS(32,3)=1HX                                                    USMAP
      DENS(33,1)=1HO                                                    USMAP
      DENS(33,2)=1H=                                                    USMAP
      DENS(33,3)=1HY                                                    USMAP
      DENS(34,1)=1HT                                                    USMAP
      DENS(34,2)=1H/                                                    USMAP
      DENS(34,3)=1HU                                                    USMAP
      DENS(35,1)=1HH                                                    USMAP
      DENS(35,2)=1H=                                                    USMAP
      DENS(35,3)=1HT                                                    USMAP
      DENS(36,1)=1HG                                                    USMAP
      DENS(36,2)=1H+                                                    USMAP
      DENS(36,3)=1HX                                                    USMAP
      DENS(37,1)=1HO                                                    USMAP
      DENS(37,2)=1H-                                                    USMAP
      DENS(37,3)=1HX                                                    USMAP
      DENS(38,1)=1HG                                                    USMAP
      DENS(38,2)=1H*                                                    USMAP
      DENS(38,3)=1HX                                                    USMAP
      DENS(39,1)=1HT                                                    USMAP
      DENS(39,2)=1HX                                                    USMAP
      DENS(39,3)=1HH                                                    USMAP
      DENS(40,1)=1HH                                                    USMAP
      DENS(40,2)=1HI                                                    USMAP
      DENS(40,3)=1HX                                                    USMAP
      DENS(41,1)=1HE                                                    USMAP
      DENS(41,2)=1HM                                                    USMAP
      DENS(41,3)=1H/                                                    USMAP
      DENS(42,1)=1HE                                                    USMAP
      DENS(42,2)=1HO                                                    USMAP
      DENS(42,3)=1H*                                                    USMAP
      DENS(43,1)=1HH                                                    USMAP
      DENS(43,2)=1HO                                                    USMAP
      DENS(43,3)=1H*                                                    USMAP
      DENS(44,1)=1H$                                                    USMAP
      DENS(44,2)=1HO                                                    USMAP
      DENS(44,3)=1HX                                                    USMAP
      DENS(45,1)=1HW                                                    USMAP
      DENS(45,2)=1HO                                                    USMAP
      DENS(45,3)=1H$                                                    USMAP
      ITABLE=15                                                         USMAP
   20 PRINT 1000,T                                                      USMAP
 1000 FORMAT(1H1,6H TIME=F15.5////)                                     USMAP
      IIP1=II+1                                                         USMAP
      IIP2=II+2                                                         USMAP
      DO 30 I=1,IIP2                                                    USMAP
   30 P(I,1)=1H*                                                        USMAP
      PRINT 1001,(P(I,1),I=1,IIP2)                                      USMAP
      DO 80 LINE=1,JJ                                                   USMAP
      J=JJ+1-LINE                                                       USMAP
      GO TO (50,50,40),KFETA                                            USMAP
   40 K=44.*C(II+1,J)+1.0001                                            USMAP
      P(1,1)=DENS(K,1)                                                  USMAP
      P(1,2)=DENS(K,2)                                                  USMAP
      P(1,3)=DENS(K,3)                                                  USMAP
      GO TO 60                                                          USMAP
   50 P(1,1)=1H*                                                        USMAP
      P(1,2)=1H*                                                        USMAP
      P(1,3)=1H*                                                        USMAP
   60 DO 70 I=1,II                                                      USMAP
      K=44.*C(I,J)+1.0001                                               USMAP
      P(I+1,1)=DENS(K,1)                                                USMAP
      P(I+1,2)=DENS(K,2)                                                USMAP
   70 P(I+1,3)=DENS(K,3)                                                USMAP
      P(II+2,1)=1H*                                                     USMAP
      P(II+2,2)=1H*                                                     USMAP
      P(II+2,3)=1H*                                                     USMAP
      PRINT 1001,(P(I,1),I=1,IIP2)                                      USMAP
 1001 FORMAT(1H ,105A1)                                                 USMAP
      PRINT 1002,(P(I,2),I=1,IIP2)                                      USMAP
 1002 FORMAT(1H+,105A1)                                                 USMAP
      PRINT 1002,(P(I,3),I=1,IIP2)                                      USMAP
   80 CONTINUE                                                          USMAP
      DO 90 I=1,IIP2                                                    USMAP
   90 P(I,1)=1H*                                                        USMAP
      PRINT 1001,(P(I,1),I=1,IIP2)                                      USMAP
      PRINT 1003                                                        USMAP
 1003 FORMAT(1H1)                                                       USMAP
      RETURN                                                            USMAP
      END                                                               USMAP
      SUBROUTINE C4ETA(I,J)                                             C4ETA2
*     SYMBOL TABLE                                                      C4ETA2
*     LABEL                                                             C4ETA2
*     LIST 8                                                            C4ETA2
C     C4ETA-2, FEB. 19, 1966.                                           C4ETA2
C     C4ETA(I,J) GIVES THE COEFFICIENTS FOR THE ETA-EQUATION            C4ETA2
C     AT THE POINT (I,J).                                               C4ETA2
C     C4ETA-2 IS FOR THE SOURCE-SINK PROBLEM.                           C4ETA2
      DIMENSION C(53,53),CSTAR(53,53),CSS(53,53)                        C4ETA2
      COMMON C,CSTAR,CSS,II,JJ,DTIME,DETA,DCSI,ALFALP,ALFATP,DMOLP,     C4ETA2
     1UZERO,ELZERO,ETAMIN,CSIMIN,EPSAB,A1,A2,A3,A4,B1,B2,B3,            C4ETA2
     2KFETA,CFETA,KLETA,CLETA,KFCSI,CFCSI,KLCSI,CLCSI,                  C4ETA2
     3ZETAE,BETAE,GAMAE,DELTA1,DELTA2,DELTA3,DELTA4,DELTA5,             C4ETA2
     4ZETAC,BETAC,GAMAC,DELTA6,DELTA7,DELTA8,DELTA9,DELT10,RO1,RO2,RO3  C4ETA2
      COSHF(ARG)=(EXPF(ARG)+EXPF(-ARG))/2.                              C4ETA2
      VELOCF(AONE,ATWO)=COSHF(AONE)+COSF(ATWO)                          C4ETA2
      DESQ=DETA*DETA                                                    C4ETA2
      DCSQ=DCSI*DCSI                                                    C4ETA2
      ETA=ETAMIN+DETA*FLOATF(I-1)                                       C4ETA2
      CSI=CSIMIN+DCSI*FLOATF(J-1)                                       C4ETA2
      VIJ=VELOCF(ETA,CSI)                                               C4ETA2
      ETA=ETA+DETA                                                      C4ETA2
      VIP1J=VELOCF(ETA,CSI)                                             C4ETA2
      ETA=ETA-2.*DETA                                                   C4ETA2
      VIM1J=VELOCF(ETA,CSI)                                             C4ETA2
      ETA=ETA+DETA                                                      C4ETA2
      CSI=CSI+DCSI                                                      C4ETA2
      VIJP1=VELOCF(ETA,CSI)                                             C4ETA2
      CSI=CSI-2.*DCSI                                                   C4ETA2
      VIJM1=VELOCF(ETA,CSI)                                             C4ETA2
      DLP=0.5*ALFALP*(VIP1J+VIJ)+DMOLP                                  C4ETA2
      DLM=0.5*ALFALP*(VIJ+VIM1J)+DMOLP                                  C4ETA2
      DTP=0.5*ALFATP*(VIJP1+VIJ)+DMOLP                                  C4ETA2
      DTM=0.5*ALFATP*(VIJ+VIJM1)+DMOLP                                  C4ETA2
      VDT=VIJ*VIJ*DTIME                                                 C4ETA2
      ZETAE=B3/VDT-DLM/DESQ-A4/DETA                                     C4ETA2
      BETAE=B1/VDT+(DLP+DLM)/DESQ+(A4-A3)/DETA                          C4ETA2
      GAMAE=B2/VDT-DLP/DESQ+A3/DETA                                     C4ETA2
      DELTA1=B3/VDT+A2/DETA                                             C4ETA2
      DELTA2=B1/VDT-(DTM+DTP)/DCSQ+(A1-A2)/DETA                         C4ETA2
      DELTA3=B2/VDT-A1/DETA                                             C4ETA2
      DELTA4=DTM/DCSQ                                                   C4ETA2
   10 DELTA5=DTP/DCSQ                                                   C4ETA2
      RETURN                                                            C4ETA2
      END                                                               C4ETA2
```

```
      SUBROUTINE C4CSI (I,J)                                            C4CSI2
*     SYMBOL TABLE                                                      C4CSI2
*     LABEL                                                             C4CSI2
*     LIST 8                                                            C4CSI2
C     C4CSI-2, FEB. 19, 1966.                                           C4CSI2
```

```
C     C4CSI(I,J) GIVES THE COEFFICIENTS FOR THE CSI-EQUATION                C4CSI2
C     AT THE POINT (I,J).                                                   C4CSI2
C     C4CSI-2 IS FOR THE SOURCE-SINK PROBLEM.                               C4CSI2
      DIMENSION C(53,53),CSTAR(53,53),CSS(53,53)                            C4CSI2
      COMMON C,CSTAR,CSS,II,JJ,DTIME,DETA,DCSI,ALFALP,ALFATP,DMOLP,         C4CSI2
     1UZERO,ELZERO,ETAMIN,CSIMIN,EPSAB,A1,A2,A3,A4,B1,B2,B3,                C4CSI2
     2KFETA,CFETA,KLETA,CLETA,KFCSI,CFCSI,KLCSI,CLCSI,                      C4CSI2
     3ZETAE,BETAE,GAMAE,DELTA1,DELTA2,DELTA3,DELTA4,DELTA5,                 C4CSI2
     4ZETAC,BETAC,GAMAC,DELTA6,DELTA7,DELTA8,DELTA9,DELT10,RO1,RO2,RO3      C4CSI2
      COSHF(ARG)=(EXPF(ARG)+EXPF(-ARG))/2.                                  C4CSI2
      VELOCF(AONE,ATWO)=COSHF(AONE)+COSF(ATWO)                              C4CSI2
      DESQ=DETA*DETA                                                        C4CSI2
      DCSQ=DCSI*DCSI                                                        C4CSI2
      ETA=ETAMIN+DETA*FLOATF(I-1)                                           C4CSI2
      CSI=CSIMIN+DCSI*FLOATF(J-1)                                           C4CSI2
      VIJ=VELOCF(ETA,CSI)                                                   C4CSI2
      CSI=CSI+DCSI                                                          C4CSI2
      VIJP1=VELOCF(ETA,CSI)                                                 C4CSI2
      CSI=CSI-2.*DCSI                                                       C4CSI2
      VIJM1=VELOCF(ETA,CSI)                                                 C4CSI2
      DTP=0.5*ALFATP*(VIJP1+VIJ)+DMOLP                                      C4CSI2
      DTM=0.5*ALFATP*(VIJ+VIJM1)+DMOLP                                      C4CSI2
      VDT=VIJ*VIJ*DTIME                                                     C4CSI2
      ZETAC=-DTM/DCSQ                                                       C4CSI2
      BETAC=B1/VDT+(DTM+DTP)/DCSQ                                           C4CSI2
      GAMAC=-DTP/DCSQ                                                       C4CSI2
      DELTA6=ZETAC                                                          C4CSI2
      DELTA7=(DTM+DTP)/DCSQ                                                 C4CSI2
      DELTA8=GAMAC                                                          C4CSI2
      DELTA9=0.                                                             C4CSI2
      DELT10=0.                                                             C4CSI2
      RO1=B1/VDT                                                            C4CSI2
      RO2=0.                                                                C4CSI2
   10 RO3=0.                                                                C4CSI2
      RETURN                                                                C4CSI2
      END                                                                   C4CSI2
```

```
      SUBROUTINE CFEXP (I,J)                                                CFEXP2
*     SYMBOL TABLE                                                          CFEXP2
*     LABEL                                                                 CFEXP2
*     LIST 8                                                                CFEXP2
C     CFEXP-2, FEB. 19, 1966.                                               CFEXP2
C     CFEXP(I,J) GIVES THE COEFFICIENTS FOR THE EXPLICIT EQUATION           CFEXP2
C     AT THE POINT (I,J).                                                   CFEXP2
C     CFEXP-2 IS FOR THE SOURCE-SINK PROBLEM.                               CFEXP2
      DIMENSION C(53,53),CSTAR(53,53),CSS(53,53)                            CFEXP2
      COMMON C,CSTAR,CSS,II,JJ,DTIME,DETA,DCSI,ALFALP,ALFATP,DMOLP,         CFEXP2
     1UZERO,ELZERO,ETAMIN,CSIMIN,EPSAB,A1,A2,A3,A4,B1,B2,B3,                CFEXP2
     2KFETA,CFETA,KLETA,CLETA,KFCSI,CFCSI,KLCSI,CLCSI,                      CFEXP2
     3ZETAE,BETAE,GAMAE,DELTA1,DELTA2,DELTA3,DELTA4,DELTA5,                 CFEXP2
     4ZETAC,BETAC,GAMAC,DELTA6,DELTA7,DELTA8,DELTA9,DELT10,RO1,RO2,RO3,     CFEXP2
     5P1,P2,P3,Q1,Q2,Q3,S1,S2,S3
      COSHF(ARG)=(EXPF(ARG)+EXPF(-ARG))/2.                              CFEXP2
      VELOCF(AONE,ATWO)=COSHF(AONE)+COSF(ATWO)                          CFEXP2
      DESQ=DETA*DETA                                                    CFEXP2
      DCSQ=DCSI*DCSI                                                    CFEXP2
      ETA=ETAMIN+DETA*FLOATF(I-1)                                       CFEXP2
      CSI=CSIMIN+DCSI*FLOATF(J-1)                                       CFEXP2
      VIJ=VELOCF(ETA,CSI)                                               CFEXP2
      ETA=ETA+DETA                                                      CFEXP2
      VIP1J=VELOCF(ETA,CSI)                                             CFEXP2
      ETA=ETA-2.*DETA                                                   CFEXP2
      VIM1J=VELOCF(ETA,CSI)                                             CFEXP2
      ETA=ETA+DETA                                                      CFEXP2
      CSI=CSI+DCSI                                                      CFEXP2
      VIJP1=VELOCF(ETA,CSI)                                             CFEXP2
      CSI=CSI-2.*DCSI                                                   CFEXP2
      VIJM1=VELOCF(ETA,CSI)                                             CFEXP2
      DLP=0.5*ALFALP*(VIP1J+VIJ)+DMOLP                                  CFEXP2
      DLM=0.5*ALFALP*(VIJ+VIM1J)+DMOLP                                  CFEXP2
      DTP=0.5*ALFATP*(VIJP1+VIJ)+DMOLP                                  CFEXP2
      DTM=0.5*ALFATP*(VIJ+VIJM1)+DMOLP                                  CFEXP2
      VDT=VIJ*VIJ*DTIME                                                 CFEXP2
      P1=1.+(A1-A2)*VDT/DETA                                            CFEXP2
      P2=A2*VDT/DETA                                                    CFEXP2
      P3=-A1*VDT/DETA                                                   CFEXP2
      Q1=DLM*VDT/DESQ+A4*VDT/DETA                                       CFEXP2
      Q2=-(DLM+DLP)*VDT/DESQ+(A3-A4)*VDT/DETA                           CFEXP2
      Q3=DLP*VDT/DESQ-A3*VDT/DETA                                       CFEXP2
      S1=DTM*VDT/DCSQ                                                   CFEXP2
      S2=-(DTM+DTP)*VDT/DCSQ                                            CFEXP2
   10 S3=DTP*VDT/DCSQ                                                   CFEXP2
      RETURN                                                            CFEXP2
      END                                                               CFEXP2
```

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APPENDIX C: DEFINITION OF SYMBOLS

A	specific discharge in radial flow $[L^2/T]$.
a_1-a_4	weighting coefficients in convective term.
b	thickness of confined aquifer.
b_1-b_3	weighting coefficients in time term.
b_1, b_2	y-coordinates of interfaces between layers.
C	concentration.
C_0	reference concentration.
C^*, C^{**}, C^{***}	intermediate values of calculated concentration.
D_{ik}	"factor of dispersion" $[L^2/T]$.
D_L	longitudinal dispersion coefficient $[L^2/T]$.
D_T	lateral dispersion coefficient $[L^2/T]$.
D_m	molecular diffusivity $[L^2/T]$.
DL	defined in equations (3-30) and (3-31).
DT	defined in equations (3-32) and (3-33).
D_m'	non-dimensional molecular diffusivity.
d_{50}	mean grain diameter of sand. $[L]$
I	number of grid points along the streamline.
i	subscript of grid points along the streamline.
J	number of grid points along the equipotential.
j	subscript of grid points along the equipotential.
k	intrinsic permeability $[L^2]$.
ℓ	length.
ℓ_0	reference length.
ℓ_x	length in x-direction.
n	subscript of time increments
P	probe resistance.
P_1-P_3	coefficients in equation (3-39).
P	dummy variable in the Laplace transform.
Q	discharge.
Q_1-Q_3	coefficients in equation (3-39).

Q_f	fresh water discharge.
Q_s	salt water discharge.
q	seepage velocity (along a streamline).
q	$= p/\alpha_L$.
$\mathbb{R}_{d_{50}}$	Reynolds number based on d_{50}.
$\mathbb{R}_{\sqrt{k}}$	Reynolds number based on k.
r	radius.
S_1-S_3	coefficients in equation (3-39).
t	time.
u	seepage velocity.
u_0	reference velocity.
V_k	temporary value for tri-diagonal matrix, equation (3-44).
v	non-dimensional seepage velocity.
W_k	temporary value for tri-diagonal.
x, y, z	Cartesian coordinates.
α_L	longitudinal dispersivity [L].
α_L'	non-dimensional α_L.
α_T	lateral dispersivity.
α_T'	non-dimensional α_T.
γ	conductance.
Δ	increment.
δ	deflection of Sanborn pen.
ϵ_{CN}	generalized Crank-Nicholson weighting coefficient in second derivative.
η	non-dimensional potential.
θ	porosity.
ν	kinematic viscosity [L^2/T].
ξ	non-dimensional stream-function.
τ	non-dimensional time.
ω	frequency.
ψ	stream function.
Φ	potential.